

NIST PUBLICATIONS

# Publications of the National Institute of Standards and Technology 1991 Catalog

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artment of Commerce
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stitute of Standards and Technology

he National Institute of Standards and Technology was established in 1988 by Congress to "assist industry in the development of technology . . . needed to improve product quality, to modernize manufacturing processes, to ensure product reliability . . . and to facilitate rapid commercialization . . . of products based on new scientific discoveries."

NIST, originally founded as the National Bureau of Standards in 1901, works to strengthen U.S. industry's competitiveness; advance science and engineering; and improve public health, safety, and the environment. One of the agency's basic functions is to develop, maintain, and retain custody of the national standards of measurement, and provide the means and methods for comparing standards used in science, engineering, manufacturing, commerce, industry, and education with the standards adopted or recognized by the Federal Government.

As an agency of the U.S. Commerce Department's Technology Administration, NIST conducts basic and applied research in the physical sciences and engineering and performs related services. The Institute does generic and precompetitive work on new and advanced technologies. NIST's research facilities are located at Gaithersburg, MD 20899, and at Boulder, CO 80303. Major technical operating units and their principal activities are listed below. For more information contact the Public Inquiries Desk, 301-975-3058.

# **Technology Services**

- Manufacturing Technology Centers Program
- Standards Services
- Technology Commercialization
- Measurement Services
- Technology Evaluation and Assessment
- Information Services

# **Electronics and Electrical Engineering Laboratory**

- Microelectronics
- · Law Enforcement Standards
- Electricity
- Semiconductor Electronics
- Electromagnetic Fields1
- Electromagnetic Technology¹

# Chemical Science and Technology Laboratory

- Biotechnology
- Chemical Engineering<sup>1</sup>
- Chemical Kinetics and Thermodynamics
- Inorganic Analytical Research
- Organic Analytical Research
- Process Measurements
- Surface and Microanalysis Science
- Thermophysics<sup>2</sup>

# **Physics Laboratory**

- Electron and Optical Physics
- Atomic Physics
- Molecular Physics
- Radiometric Physics
- Quantum Metrology
- · Ionizing Radiation
- Time and Frequency<sup>1</sup>
- Quantum Physics<sup>1</sup>

# Manufacturing Engineering Laboratory

- Precision Engineering
- Automated Production Technology
- Robot Systems
- Factory Automation
- Fabrication Technology

# Materials Science and Engineering Laboratory

- Intelligent Processing of Materials
- Ceramics
- Materials Reliability¹
- Polymers
- Metallurgy
- Reactor Radiation

# **Building and Fire Research Laboratory**

- Structures
- Building Materials
- Building Environment
- · Fire Science and Engineering
- Fire Measurement and Research

# **Computer Systems Laboratory**

- Information Systems Engineering
- Systems and Software Technology
- Computer Security
- Systems and Network Architecture
- Advanced Systems

# Computing and Applied Mathematics Laboratory

- Applied and Computational Mathematics<sup>2</sup>
- Statistical Engineering<sup>2</sup>
- Scientific Computing Environments<sup>2</sup>
- Computer Services<sup>2</sup>
- Computer Systems and Communications<sup>2</sup>
- Information Systems

<sup>&</sup>lt;sup>1</sup>At Boulder, CO 80303.

<sup>&</sup>lt;sup>2</sup>Some elements at Boulder, CO 80303.

# Publications of the National Institute of Standards and Technology 1991 Catalog

Ernestine T. Gladden, Editor

Office of Information Services National Institute of Standards and Technology Gaithersburg, MD 20899

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## CATALOG STRUCTURE AND USE

Full bibliographic citations including keywords and abstracts for National Institute of Standards and Technology (NIST) papers published and entered into the National Technical Information Service (NTIS) collection are cited in the "NIST Publications Announcements" section of this catalog. (Also included are papers published prior to 1991 but not reported in previous supplements of this annual catalog.) Entries are arranged by NTIS subject classifications which consist of 38 broad subject categories (see back cover) and over 350 subcategories. Within a subcategory, entries are listed alphanumerically by NTIS order number.

Four indexes are included to allow the user to identify papers by personal author, keywords, title, and NTIS order/report number. Each entry lists the appropriate title, the NTIS order number, and the abstract number.

Papers may also be identified by searching the NTIS database either online via commercially available systems such as DIALOG, or in the issues of NTIS's Government Reports Announcements and Index and its Government Reports Annual Index.

#### AVAILABILITY AND ORDERING INFORMATION

The highest quality and least expensive copies of NIST publications published as Government documents are available from the Superintendent of Documents, U.S. Government Printing Office, Washington, DC 20402. Publications cited with stock numbers (SN) should be ordered by these numbers. GPO will accept payment by check, money order, VISA, MasterCard, or deposit account. For availability and price, write to the GPO or telephone (202) 783-3238. Should an NIST publication be out of print at the GPO, its continued availability is assured at NTIS which sells publications in microfiche or paper copy reproduced from microfiche.

If an entry has a price code, such as PC A04/MF A01, the publication may be ordered from NTIS in paper copy (PC) or microfiche (MF) or both if both codes are given. Order from the National Technical Information Service, 5285 Port Royal Road, Springfield, VA 22161. A copy of the latest price code schedule is available from NTIS. NTIS will accept payment by check, money order, VISA, American Express, MasterCard, or deposit account. NTIS is the sole source of Federal Information Processing Standards (FIPS), Interagency Reports (IRs), and Grant/Contract Reports (GCRs). For more information call (703) 487-4650.

Papers noted "Not Available NTIS" may be obtained directly from the author or from the external publisher

cited. Such papers are not for sale by either the GPO or NTIS.

Two other sources for NIST publications are depository libraries (libraries designated to receive Government publications) and Department of Commerce District Offices. The depository libraries listed in Appendix A receive selected NIST publications (see inside back cover for a description of the various NIST publication series). While not every Government publication is sent to all depository libraries, certain depositories designated as Regional Depositories receive and retain one copy of all Government publications made available. Contact the depository library in your area to obtain information on what is available and where.

Department of Commerce District Offices listed in Appendix B provide ready access at the local level to publications, statistical data and summaries, and surveys. Each District Office serves as an official sales agency of the Superintendent of Documents, U.S. Government Printing Office. A wide range of Government publications can be purchased from these offices. In addition, the reference library of each District Office contains review copies of many Government publications.

# NIST PUBLICATIONS ANNOUNCEMENTS

# SAMPLE ENTRY

**ENVIRONMENTAL** CONTROL

**POLLUTION &** 

Air Poliution & Control

100.905

PC A03/MF A01 PB91-167353

National Inst. of Standards and Technology (BFRL),

Gaithersburg, MD.

**Proposed Standard Practice for Assessing the** 

Performance of Gas-Phase Air Cleaning Equipment

S. Silberstein, Mar 91, 23 p

NISTIR-4523

Contract F-000000

Key words: \*Indoor air pollution \*Air cleaners, \*Air pollution control equipment, \*Standards, Air flow, Activated carbon, Service life, Air filters, Performance, Contaminants, Airborne wastes.

The proposed standard practice provides a general and flexible laboratory method for assessing the performance of equipment for controlling indoor concentrations of gas-phase air contaminants. Using a canister filled with adsorption media, a profile of breakthrough concentration over time is obtained during each test conducted at a fixed contaminant challenge concentration. Results of tests performed for different contaminants and different challenge concentrations can be used for estimating the useful life of air cleaning equipment, and for comparing equipment. The Information will be useful to the engineer for the design and selection of such equipment.

**NTIS Subject Category** 

**NTIS Subcategory** 

Abstract Number

NTIS order number Availability Price Codes

Corporate or performing organization

Report Title

Personal authors

Report date

Page count

Report Number

Contract or grant number

Keywords: \* Indicates keyword index entry

Abstract

# **ADMINISTRATION &** MANAGEMENT

#### **Management Practice**

100 001

PC A05/MF A01 PB91-167833 National Inst. of Standards and Technology, Gaithers-

Interim Report to the President and to the Congress on the Malcolm Baldrige National Quality Award.

Interim rept. (Final).

Apr 91, 90p
Portions of this document are not fully legible. This publication does not have a series number assigned.

Keywords: \*Quality control, \*Awards, United States, Productivity, Small business, Manufacturers, Indus-

tries, Information transfer, \*Quality management, Malcolm Baldrige National Quality Award.

Contents: A Note from the Secretary; Acknowledgments; Executive Summary; The Malcolm Baldrige National Quality Improvement Act of 1987: Background and Purposes; Award Program Design; 1988 Award Program; 1989 Award Program; 1990 Award Program; Progress in Information Transfer; Benefits of the Award Program; Implications of the Award: Strengthening U.S. Competitiveness; Key Issues; Findings and Conclusions; Appendices.

100,002

PB92-126481 PC A03/MF A01 National Inst. of Standards and Technology, Gaithers-

Feasibility of Using a Multiple Award Schedule for Specifying Paints in Government Painting Con-

tracts.
M. E. McKnight. Nov 91, 19p NISTIR-4706
See also PB86-230653. Sponsored by Tri-Services Facilities Coatings Committee.

Keywords: \*Government procurement, \*Contracts, \*Awards, Painting, Coatings, General Services Administration.

The Department of Defense is placing increasing emphasis on the use of commercially available or brand-

ed products in lieu of Military or Federal Specification products in building construction and maintenance. However, there are few industry consensus specifica-tions for paints and coatings. Although non-government consensus coating specifications are being developed, a General Services Administration Federal Supply Schedule provides an additional mechanism through which Federal agencies can obtain commercially available coatings. Specifically, the use of a Multiple Award Federal Supply Schedule in a military painting contract is discussed in the report. Procedures for obtaining the lowest cost metric the vertical that would dures for obtaining the lowest cost material that would meet the Government's minimum needs are ad-dressed. A description of need based upon perform-ance criteria for the specific end use, that would be included in a painting contract, is suggested. Advantages and disadvantages of using a Multiple Award Schedule in painting contracts are enumerated. Advantages include providing a mechanism for using new coating technology, taking advantage of manufactur-er's technical support and knowledge of regulatory issues, and decreasing the need for revising or preparing new coating specifications. Disadvantages include the additional effort needed to revise guide specifications, train both coating users and suppliers in new procedures and the lack of performance criteria for some end uses. Despite the disadvantages cited, it is concluded that the advantages outweigh the disadvantages and that use of a Multiple Award Schedule in painting contracts is feasible.

#### **ADMINISTRATION & MANAGEMENT**

# Personnel Management, Labor Relations & Manpower Studies

#### Personnel Management, Labor Relations & Manpower Studies

100.003

PB91-231555 PC A05/MF A01 National Inst. of Standards and Technology, Gaithersburg, MD. Office of Personnel and Civil Rights.

NIST Personnel Management Description

Personnel Management Demonstration Project: Design, Implementation and Accomplish-

A. Cassady. Jul 91, 94p NISTIR-4640

Keywords: \*Personnel management, \*Payment systems, Government employees, Compensation, Income, Employment, Performance evaluation, Per-Classification, Demonstration formance standards, Classification, Demonstration projects, Managers, \*National Institute of Standards and Technology.

The NIST Authorization Act for Fiscal Year 1987 provided for a 5-year project to demonstrate an alterna-tive personnel management system, which was implemented January 1, 1988. The project system was built on the concepts of total compensation comparability, market sensitivity, pay for performance, administrative simplicity, management flexibility, and governmentwide applicability. Designed to improve hiring and re-tention of high-quality personnel and to more effective-ly compensate and retain high performers, the project dramatically changed the way NIST administers pay, position classification, recruitment, qualifications examination, retention, and performance management for former General Schedule employees. Evaluations and feedback from managers and employees have shown that project personnel systems have improved NIST's ability to recruit and retain quality staff; make compensation more competitive; link pay to performance; simplify position classification; streamline processing; improve the staffing process and get new hires aboard faster; and increase the manager's role and accountability in personnel management.

#### **Productivity**

100.004

PB91-177774 PC A99/MF A04 National Inst. of Standards and Technology, Gaithersburg, MD. Office of Standards Code and Information. Standards Activities of Organizations in the United States.

Special pub. (Final). R. B. Toth. Feb 91, 738p NIST/SP-806 Supersedes PB85-106151. Also available from Supt. of Docs. See also PB89-221147.

Keywords: \*Standardization, \*Organizations, \*United States, \*Directories, Standards, Trade associations, Sources, National government, Specifications, Military organizations, Technical societies, Recommenda-

The directory is a guide to mandatory and voluntary standards activities in the United States at the national level - both governmental and nongovernmental (trade associations, technical and other professional societies). It excludes proprietary (company standards) and state and local levels of government (i.e., county and municipal). It supersedes the 1984 edition (NBS SP 681), 'Standards Activities of Organizations in the United States.' It includes standards distributors, libraries, and information centers, and union lists of standards repositories by regional areas. It also lists organizations that no longer develop standards. Over 750 current descriptive commentaries are formatted, with subject headings to facilitate access to specific infor-mation. The main sections cover nongovernment; fed-eral government; sources of standards documents and information; a subject index and related listings covering acronyms and initials, defunct bodies, and those organizations with name changes. Organizations have been included if they develop standards or contribute to the standardization process, whether voluntary or mandatory, or are sources of standards documents or information. An introductory section provides general information on federal (including military) standards activities, a list of 20 major nongovernment standards developers, some historical notes, and an overview of U.S. (national) standardization activities.

#### **Public Administration & Government**

100.005 PB91-167379 PC A06/MF A01 National Inst. of Standards and Technology, Gaithersburg, MD. Office of Standards Code and Information. Directory of Federal Government Laboratory Accreditation/Designation Programs.

Special pub. (Final).
M. Breitenberg. Feb 91, 105p NIST/SP-808
Also available from Supt. of Docs. See also PB88-

Keywords: \*Laboratories, \*Certification, \*Directories, Specifications, Regulations, Standards, Inspection, Grading, Data bases, \*Federal Government certification, Approved products.

The directory is designed to provide updated information on federal government laboratory accreditation and similar type programs conducted by the federal government. The programs designate a set of labora-tories or other entities to conduct testing to assist federal agencies in carrying out their responsibilities. The programs include an assessment regarding the capability of the laboratory to conduct the testing. The type and degree of such assessments, however, vary greatly by program. It should be noted that the entries in the directory are based primarily on information provided by the federal agency and reflect the agency's view of its activities. The directory is part of ongoing NIST efforts to establish and maintain comprehensive databases on standards, regulations, laboratory accredita-tion and certification programs and related information in accordance with the requirements of the Trade Agreements Act of 1979. The material has been com-piled to meet the needs of government, industry, and the public for information on U.S. Government laboratory accreditation and related programs.

100,006 PB91-222695 PC A05/MF A01 National Inst. of Standards and Technology (BFRL), Gaithersburg, MD.
Standards for the Physical Protection of National Resources and Facilities.

Final rept.
R. D. Dikkers. Jul 91, 89p NISTIR-4618
Contract IAA-EMW-90-E-3279
Sponsored by Federal Emergency Management
Agency, Washington, DC.

Keywords: \*Federal buildings, \*Security, \*Standards, Federal agencies, Equipment, Safety engineering, National government, Facilities, Area security, \*Federal Emergency Management Agency.

The specific objectives of the study are: (1) to identify and compile existing standards and guidelines pertaining to the physical protection of facilities and resources; and (2) to prepare a plan and strategies for developing national standards which may be needed to assist Federal departments and agencies in the protection of their facilities and resources

#### Research Program Administration & **Technology Transfer**

PB91-187559 PC A03/MF A01 National Inst. of Standards and Technology, Gaithersburg, MD. NIST Research Reports, March 1991.

Special pub.

Also available from Supt. of Docs. as SN003-003-03081-3. See also PB91-112813.

Keywords: \*Research, International trade, Federal budgets, High temperature superconductors, Electric contacts, Grants, Technology transfer, Drugs, Chemical analysis, Telecommunication, Polymer matrix composites, Helmets, Integrated circuits, MMIC, US NIST, Advanced Technology Program, Integrated Services Digital Network.

Contents: Research Update; America's Technology Opportunities; 1992 Budget Seeks Increase for NIST; Making Good Contact; Grants to Advance Key Industrial Technologies; Helping Companies Up the Technology Ladder; New Instrument Promises Improved

Tracking of Drugs; Call of the Future; A New Generation of Materials; Manufacturers, Skiers Gain Competitive Edge; Microwaves on a Chip; New Publications; Conference Calendar.

100,008

PB91-195545 Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Office of Energy-Related Inventions.

Trends in Technological Innovation.

Final rept.

H. Robb. 1988, 4p Sponsored by American Society of Mechanical Engineers, New York.

Pub. in Proceedings of the Intersociety Energy Conversion Engineering Conference (23rd), Denver, CO., July 31-August 5, 1988, p305-308.

Keywords: \*Technology innovation, \*Trends, Research and development, Technology utilization, Inventions, Changes, Industries, Manufacturing, Businesses, Reprints.

In the last twelve years, several trends have begun to emerge with respect to the type of inventor and the type and level of technology that have succeeded and will succeed (or fail) in the commercial marketplace. The rate of change taking place in almost all areas of technology is not just accelerating, it is amazing. It goes without saying that the kinds of technological changes that are taking place are affecting the future of almost all manufacturing industries. In addition, even many institutions in non-technological areas, including some that seem far removed, are being affected by the rate of technological change. For instance, it is interesting to note that in the specific case of banking the rate of change in technological development throughout the general scientific community is affecting them in ways that many in the banking industry seem to not be aware of. Yet, these many technological developments are quietly restructuring their industry, from the outside. Similar trends are underway in most areas of business

100.009

PB91-204032 Not available NTIS National Bureau of Standards (IMSE), Gaithersburg,

Advanced Materials: Opportunities and Challenges.

L. H. Schwartz. 1988, 8p Pub. in Proceedings of Israel Materials Engineering Conference (4th), Beer Sheva, Israel, December 7-8, 1988. p51-58.

Keywords: \*Materials, \*Process control, \*Research projects, \*Data bases, Polymers, Mechanical proper-ties, Cost analysis, Intermetallic compounds, Design criteria, Composite materials, Ceramics, Reprints, Research needs.

Advanced materials include high performance composites, fine ceramics, intermetallic alloys, and advanced polymers. All technologically developed na-tions have identified these advanced materials along with biotechnology and information technology as the three principal emerging technologies for the next several decades. However, several obstacles must be overcome before the laboratory promise of advanced materials can be converted into practical, economically attrative alternatives to existing materials. Principal among these obstacles are: the demanding process control required to achieve an adequate level of reproducible quality at low cost; the push from international competitors leading to simultaneous rather than sequential development of processing, structure characterization, properties evaluation and performance as-sessment, the increased variety of materials available for a given application requiring the development of engineering property data bases.

100 010

PB91-206748 PC A03/MF A01 National Inst. of Standards and Technology, Gaithers-burg, MD. National Voluntary Lab. Accreditation Pro-

gram.
NVLAP FY 90 Annual Report.
V. R. White. Jun 91, 19p NISTIR-4599 See also PB90-198920.

Keywords: \*Laboratories, \*Certification, Project management, Research management, Reports, Test facilities, Personnel, Information systems, Research

## Research Program Administration & Technology Transfer

projects, Organizational structure, Programs, \*NVLAP(National Volunteer Laboratory Accreditation Program).

The report summarizes activities of the National Voluntary Laboratory Accreditation Program (NVLAP) for the fiscal year which ended September 30, 1990. The report covers NVLAP Operations, Technical Activities, Staffing, Publications, Talks and Presentations. The Technical Activities section presents individual descriptions of areas of new activity in FY 90 (Airborne Asbestos Analysis, Secondary Calibration for Ionizing Radiation, Plumbing, GOSIP, POSIX, Fasteners, and Calibration), as well as a summary of future program developments.

PB91-216531 PC A20/MF A04
National Inst. of Standards and Technology (TS),
Gaithersburg, MD. Information Resources and Serv-PC A20/MF A04

**Publications of the National Institute of Standards** and Technology, 1990 Catalog. Rept. for Jan-Dec 90.

T. Gladden. Jun 91, 463p NIST/SP-305-SUPPL-22

Also available from Supt. of Docs. as SN003-003-03085-6. See also PB90-271818.

Keywords: \*Catalogs(Publications), \*Bibliographies, Science, Technology, Research management, \*National Institute of Standards and Technology.

Full bibliographic citations including keywords and abstracts for National Institute of Standards and Technology (NIST) (formerly National Bureau of Standards (NBS)) papers published and entered into the National Technical Information Service (NTIS) collection are cited in the 'NIST Publications Announcements' section of the catalog. Entries are arranged by NTIS subject classifications which consist of 38 broad subject categories and over 350 subcategories. Within a subcategory, entries are listed alphanumerically by NTIS order number. Four indexes are included to allow the user to identify papers by personal author, keywords, title, and NTIS order/report number. Each entry lists the appropriate title, the NTIS order number, and the abstract number.

100,012 PB92-109172 PC A05/MF A01 National Inst. of Standards and Technology, Gaithersburg, MD. Public Affairs Div.

Research. Services. Facilities. (National Institute of Standards and Technology).

Special pub. M. A. Bello, G. Porter, and S. A. Shaffer, Aug 91, 92p NIST/SP-817

Also available from Supt. of Docs.

Keywords: \*Research facilities, \*Research programs, US NBS, Cooperation, Government/industry relations, \*National Institute of Standards and Technology, US

Each year more than 1,000 researchers from industry, universities, or other government agencies come to NIST to conduct cooperative research projects lasting from a few weeks to several years. The document describes the full spectrum of NIST programs and facilities available for industry participation and use. Each item includes the name and phone number of a NIST program manager or researcher to contact for more information. Contents: Gaining the competitive edge; Serving the customer; Technology services; Electron-Serving the customer; I echnology services; Electron-ics and Electrical Engineering Laboratory; Manufactur-ing Engineering Laboratory; Chemical Science and Technology Laboratory; Physics Laboratory; Materials Science and Engineering Laboratory; Building and Fire Research Laboratory; Computer Systems Laboratory; Computing and Applied Mathematics Laboratory; Fa-cilities index; Subject index.

100,013 PB92-126697

(Order as PB92-126614, PC A06/MF A02) National Inst. of Standards and Technology, Gaithersburg, MD.

Advanced Technology Program: A New Role for NIST in Accelerating the Development of Commercially Important Technologies.

B. C. Belanger, G. A. Uriano, and R. G. Kammer. 1991, 7p

Included in Jnl. of Research of the National Institute of Standards and Technology, v96 n5 p605-611 Sep/Oct Keywords: \*Technology, Joint ventures, Competition, Selection, Awards, \*Advanced Technology Program, ATP program, Competitiveness, US NIST

The Advanced Technology Program (ATP) is a new extra mural program operated by the National Institute of Standards and Technology (NIST) for the Department of Commerce's Technology Administration. The ATP will help enhance U.S. competitiveness by funding the development of pre-competitive, generic tech-nologies in partnership with industry. The paper de-scribes the ATP, the first ATP awards made by NIST, and the prognosis for the success of the ATP.

of other investigations reported in the literature are discussed which support the conclusions of the work. The relationship between the centerline mixing and entrainment behaviors of these flows is explored.

# **AGRICULTURE & FOOD**

# **AERONAUTICS & AERODYNAMICS**

#### **Aerodynamics**

PB92-117183 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Fire Measurement and Research

Effects of Global Density Ratio on the Centerline Mixing Behavior of Axisymmetric Turbulent Jets. Final rept.

W. M. Pitts. 1991, 10p Contract AFOSR-ISSA-85-00012 See also PB87-225413. Sponsored by Air Force Office of Scientific Research, Bolling AFB, DC. Pub. in Experiments in Fluids 11, p125-134 1991.

Keywords: \*Density ration, \*Jet mixing flow, \*Concentration(Composition), \*Turbulent flow, Mixing, Turbulence, Light scattering, Gas flow, Rayleigh scattering, Density(Mass/Volume), Density measurement,

Measurements, utilizing Rayleigh light scattering, of time-averaged concentration and unmixedness have been made along the centerlines of axisymmetric turbulent jets formed from six pairs of jet and ambient gases. Jet to ambient density ratios range from 0.14 to 5.11. Findings are compared with predictions of an approx. similarity analysis and with extensive previous literature measurements. It is shown that virtual origins for plots of inverse time-averaged concentration are strongly dependent on global density ratio. Unmixedness values first grow with increasing distance from the jet source and then achieve an asymptote. The flow distance required to reach this asymptote is a strong function of density ratio.

PB92-117209 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Fire Measurement and Research

Reynolds Number Effects on the Mixing Behavior of Axisymmetric Turbulent Jets.

W. M. Pitts. 1991, 7p Contract AFOSR-ISSA-85-00012

See also PB87-201836. Sponsored by Air Force Office of Scientific Research, Bolling AFB, DC. Pub. in Experiments in Fluids 11, p135-141 1991.

Keywords: \*Reynolds number. \*Concentration(Composition), \*Jet mixing flow, \*Turbulent flow, Mixing, Turbulence, Light scattering, Gas flow, Rayleigh scattering, Propane, Carbon tetrafluoride, Sulfur hexafluoride, Jets, Reprints.

Measurements of time-averaged jet fluid mass fraction and unmixedness are reported along the centerlines of axisymmetric jets having Reynolds numbers (Re) cov-ering a range of 3,950-11,880. Jet gases investigated are propane, carbon tetrafluoride, and sulfur hexafluor-ide. The slopes for the fall off of inverse centerline mass fraction with distance are found to be independent of Re for moderate downstream distances, but virtual origins for the data are shown to move downstream with increasing Re. Unmixedness measurements show that flows with higher Re require longer flow distances to achieve asymptotic behavior. Results

## Food Technology

100,016

PB91-150060 Not available NTIS National Inst. of Standards and Technology (NML),

gamma-Irradiated Seafoods: Identification and Dosimetry by Electron Paramagnetic Resonance Spectroscopy.

Final rept. M. F. Desrosiers. 1989, 5p

Pub. in Jnl. of Agricultural and Food Chemistry 37, n1 p96-100 Jan/Feb 89.

Keywords: \*Seafood, \*Food processing, Electron spin resonance, Aquatic animals, Dosimetry, Free radicals, Cobalt 60, Acetylglucosamine, Bones, Reprints, \*Food

Electron paramagnetic resonance (EPR) spectroscopy was used to measure the production of free radicals induced by (60)Co Gamma-rays in shrimp exoskeleton, mussel shells, and fish bones. The EPR spectrum for irradiated shrimp shell was dose dependent and appeared to be derived from more than one radical. The major component of the radiation-induced spectrum resulted from radical formation in chitin, assigned by comparison with irradiated N-acetyl-D-glucosamine. Other measurements include the total yield of radicals formed as a function of dose and the longevity of the radiation-induced EPR signal. Similar measurements were made for mussel shells and fish bones, and the results are compared and discussed. It was concluded that irradiated shrimp (with shell attached) could defi-nitely be identified by this technique; however, precise determination of absorbed dose was less straightforward. Positive identification of irradiated fish bones was also clearly distinguishable, and dosimetry by EPR appeared to be feasible.

100.017

PB91-194720 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Ionizing Radiation Div. Co-Trial on ESR Identification and Estimates of

gamma-Ray and Electron Absorbed Doses Given to Meat and Bones.

Final rept.
M. F. Desrosiers, W. L. McLaughlin, L. A. Sheahen,
N. J. F. Dodd, J. S. Lea, J. C. Evans, C. C.
Rowlands, J. J. Raffi, and J. P. L. Agnel. 1990, 10p
Pub. in International Jnl. of Food Science and Technology 25, p682-691 1990.

Keywords: \*Gamma rays, \*Food processing, \*Meat, \*Bones, Electron spin resonance, Poultry, Frogs, Pork, Interlaboratory comparisons, Reprints, \*Food irradia-

A multinational co-trial was organized to determine if electron spin resonance (ESR) spectroscopy could be used to monitor foods exposed to ionizing radiation. The bones of chicken legs, frog legs and pork rib bones were prepared and distributed as unknowns to the participating laboratories. In every instance, non-irradiated bones were correctly identified as such. Moreover, irradiated bones were not only correctly identified, but relatively good estimates of the absorbed dose were obtained. An intercomparison of the different approaches used by each laboratory is discussed, and recommendations for future trials are presented.

100.018

PB92-116672 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Ionizing Radiation Div.

#### AGRICULTURE & FOOD

#### Food Technology

Electron Spin Resonance for Monitoring Radiation-Processed Meats Containing Bone. Final rept.

M. F. Desrosiers, 1991, 2p

Pub. in Jnl. of Food Science 56, n4 p1104-1105 1991.

Keywords: \*Food processing, \*Meat, \*Electron spin resonance, \*Ionizing radiation, Free radicals, Dose-response relationships, Food industry, Reprints.

Electron spin resonance (ESR) spectroscopy assessed the dose absorbed by radiation-processed meats (containing bone). Additive re-irradiation of the bone generated a dose response curve which could then be used to assess the initial dose from irradiation. An exponential fit to the ESR response to absorbed dose provided a good estimate of initial dose and was a reasonable physical description of the response from absorption of ionizing radiation by bone. These data have implications for regulation of the industry.

# **ASTRONOMY &** ASTROPHYSICS

#### **Astrophysics**

100,019 PB91-148825 Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Quantum Physics Div.

Modelling the Coronae and Chromospheres of RS CVn Systems by the Analysis of Ultraviolet, X-ray and Radio Observations.

Final rept.

J. L. Linsky. 1990, 13p Contracts NASA-NAG5-82, NASA-H-80531-B Sponsored by National Aeronautics and Space Administration, Washington, DC. Pub. in Active Close Binaries, p747-759 1990

Keywords: \*Stars, Astronomical models, Stellar chromospheres, Stellar coronal, Ultraviolet spectra, Radio spectra, X ray spectra, Binary stars, Reprints.

The author summarizes the present status of chromospheric and coronal models of active stars in RS CVn systems. The first generation models which assumed plane-parallel, one-component layers are now being supplanted by second generation models in which the covering fraction of the plage or flare plasma is esti-mated by a Doppler-imaging analysis. Third generation models should include the magnetic field geometry and the total energy balance in a self-consistent manner.

100,020 PB91-148833 Not available NTIS National Bureau of Standards (NML), Boulder, CO.

National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
Ultraviolet, Optical, Infrared, and Microwave Observations of HR 5110.
Final rept.

I. R. Little-Marenin, T. Simon, T. R. Ayres, N.

Cohen, P. A. Feldman, J. L. Linsky, and S. J. Little. 1986, 11p Contract NAG5-82

Sponsored by National Aeronautics and Space Administration, Washington, DC. Pub. in Astrophysical Jnl. 303, n2 p780-790, 15 Apr 86.

Keywords: \*Binary stars, Ultraviolet spectra, Infrared spectra, Microwave spectra, Optical spectra, Late stars, Reprints, \*HR 5110 stars, Algol type stars.

HR 5110 is a close binary system which is viewed nearly pole-on ( $i=13\,\text{deg}$ ). A comparison of the characteristics of Algol and RS CVn systems to those of HR 5110 shows that HR 5110 can also be considered an Algol system. Because the primary star is relatively cool (F2 IV) and there is no apparent emission from an accretion disk, that authors are able to detect in IUE spectra the emission of an active chromosphere and transition region of the cooler (KO IV) secondary. HR 5110 is important because it is the only known Algol system for which the properties of the secondary star can be studied in detail.

100,021 PB91-148957 Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Quantum Physics Div. Studies of H I and D I in the Local Interstellar

Medium. Final rept.

J. Murthy, R. C. Henry, H. W. Moos, A. Vidal-Madjar, J. L. Linsky, and C. Gry. 1990, 6p Pub. in Astrophysical Jnl. 356, n1 p223-228, 10 Jun 90.

Keywords: \*Interstellar matter, Ultraviolet spectra, Lyman alpha radiation, Emission spectra, Late stars, Hydrogen, Deuterium, Abundance, IUE, Reprints, Capella star.

The authors present high-dispersion IUE spectra of the hydrogen Ly(alpha) chromospheric emission line of two nearby late-type stars, Capella and lambda. Both interstellar H 1 and D 1 Ly(alpha) absorption can be seen against the chromospheric line, and the authors have derived the density, velocity dispersion, and bulk velocity of the gas in those lines of sight. They have also placed limits on the D/H ratio.

100,022 PB91-148965 Not available NTIS National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.

Spatially Resolved Flares in RS CVn Systems.

J. E. Neff, and J. L. Linsky. 1988, 4p Sponsored by National Aeronautics and Space Admin-istration, Washington, DC.

Pub. in Activity in Cool Star Envelopes, p175-178 1988.

Keywords: \*Binary stars, \*Stellar flares, Stellar chromospheres, Ultraviolet spectra, Emission spectra, Magnesium, Reprints.

The authors have isolated Mg II k emission line profiles arising solely from the flaring region during flares on AR Lac and V 711 Tau. From several high-resolution spectra obtained during the lifetime of the flare, they have determined the size and position of the flaring regions and studied the decay of the emission line width, radial velocity, and integrated line flux.

100,023 PB91-149021 Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Quantum Physics Div.

Terminal Velocities for a Large Sample of O Stars, B Supergiants, and Wolf-Rayet Stars. Final rept.

R. K. Prinja, M. J. Barlow, and I. D. Howarth. 1990, Pub. in Astrophysical Jnl. 361, p607-620, 1 Oct 90.

Keywords: \*Early stars, \*Wolf-Rayet stars, \*Supergiant stars, \*O stars, \*Stellar winds, Stellar mass ejection, Terminal velocity, Reprints, Mass loss.

The authors argue that easily measured, reliable esti-mates of terminal velocities for early-type stars are provided (1) by the central velocity asymptotically approached by narrow absorption features and (2) by the violet limit of zero residual intensity in saturated P Cygni profiles. They use these estimators to determine Cygni profiles. They use these estimators to determine terminal velocities, nu(infinity) for 181 O stars, 70 early B supergiants, and 35 Wolf-Rayet stars. For OB stars their values are typically 15%-20% smaller than the extreme violet edge velocities, nu(edge), while for WR stars, nu(infinity). 76nu(edge) on average. The authors give new mass-loss rates for WR stars which are thermal radio emitters, taking into account the authors' new terminal velocities and recent revisions to estinew terminnal velocities and recent revisions to estimates of distances and to the mean nuclear mass per electron. The authors examine the relationships between nu(infinity) the surface escape velocities, and effective temperatures.

100.024 PB91-149286 Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Quantum Physics Div. New Radio Detectors of Early-Type Pre-Main Sequence Stars.

Final rept. S. L. Skinner, A. Brown, and J. L. Linsky. 1990, 4p Pub. in Astrophysical Jnl. 357, pl.39-L42, 10 Jul 90.

Keywords: \*Pre-main sequence stars, \*Early stars, Radio sources(Astronomy), Reprints, Very large array.

The authors present results of VLA radio continuum observations of 13 early-type pre-main-sequence stars selected from the 1984 catalog of Finkenzeller and Mundt. The stars HD 259431 and MWC 1080 were detected at 3.6 cm, while HD 200775 and TY CrA were detected at both 3.6 and 6 cm. The flux density Sv of HD 200775 has a frequency dependence of the form S(sub nu) varies as nu(sup 0.50 + or - 0.3), consistent with the behavior expected for free-free emission origi-nating in a fully ionized wind. However, an observation in A configuration suggests that the source geometry in A configuration suggests that the source geometry may not be spherically symmetric. In contrast, the spectral index of TY CrA is negative with a flux behavior of the form S(sub nu) varies as nu(sup -0.15 + or -0.1), implying nonthermal emission. The physical mechanism responsible for the nonthermal emission has not yet been identified, although gyrosynchrotron and synchrotron processes cannot be ruled out.

Not available NTIS PB91-149849 National Inst. of Standards and Technology (NML), Boulder, CO. Quantum Physics Div.

Photospheres of Hot Stars. 4. Spectral Type O4. Final rept. B. Bohannan, S. A. Voels, D. G. Hummer, and D. C.

B. Bonannan, S. A. Voeis, D. G. Hallinner, and D. S. Abbott. 1990, 9p Contract NAGW-766, Grant NSF-AST85-05919 See also PB89-202592. Sponsored by National Aeronautics and Space Administration, Washington, DC., and National Science Foundation, Washington, DC. Pub. in Astrophysical Jnl. 365, p729-737, 20 Dec 90.

Keywords: \*Hot stars, Main sequence stars, Supergiant stars, O stars, Stellar atmospheres, Stellar temperature, Stellar evolution, Reprints.

The basic stellar parameters of a supergiant (zeta Pup) and two main-sequence stars, 9 Sgr and HD 46223, at spectral class O4 are determined using line profile analysis. The stellar parameters are determined by comparing high signal-to-noise hydrogen and helium line profiles with those from stellar atmosphere models which include the effect of radiation scattered back onto the photosphere from an overlying stellar wind, an effect referred to as wind blanketing. At spectral class O4, the inclusion of wind-blanketing in the model atmosphere reduces the effective temperature by an average of 10%. The shift in effective temperature is also reflected by shifts in several other stellar parameters relative to previous O4 spectral-type calibrations. It is also shown through the analysis of the two O4 V stars that scatter in spectral type calibrations is intro-duced by assuming that the observed line profile re-flects the photospheric stellar parameters.

PB91-158956 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Atomic and Plasma Radiation Div. Working Group 1: Atomic Spectra and Wavelength Standards. Final rept.

W. C. Martin. 1988, 7p

Pub. in Transactions of the International Astronomical Union, vXXA p111-117 1988.

Keywords: \*Atomic spectroscopy, Atomic energy levels, Wavelengths, Bibliographies, Reprints.

The bibliographic report describes atomic spectroscopic research and data of interest for astronomy. It covers the past 3 years.

100,027 PB91-174664 Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Quantum Physics Div.
Radio-Continuum Observations of a Variety of Cool Stars.

S. A. Drake, J. L. Linsky, P. G. Judge, and M. Elitzur. 1991, 7p

Pub. in Astronomical Jnl. 101, n1 p230-236 Jan 91.

Keywords: \*Radio sources(Astronomy), \*Cool stars, Main sequence stars, Supergiant stars, Giant stars, Radio astronomy, Stellar winds, Reprints.

The authors present radio-continuum observations made at 2 and/or 6 cm of 26 cool stars (FO and later), including 10 F-K main-sequence stars and 16 F-M giant and supergiant stars. The data were obtained as part of several Very Large Array observing programs. 22 of the observed stars were not detected as sources and have typical 3 sigma upper limits of about 0.35 mJy at 2 cm and about 0.15-0.60 mJy at 6 cm.

100,028 PB91-174920 Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Quantum Physics Div.

Detection of an Expanding H I Shell in the Old Supernova Remnant CTB 80.

Final rept.

J. M. Shull. 1990, 9p

Sponsored by National Science Foundation, Washington, DC.

Pub. in Astrophysical Jnl. 364, n1 p178-186, 20 Nov

Keywords: \*Supernova remnants, \*Nebulae, Expansion, Pulars, Reprints.

The authors have detected an expanding H I shell around the supernova remnant (SNR) CTB 80. The H I shell is clumpy and partially complete, with its SW portion opened. The shell has an expansion velocity of 72 km/s, a radius of 19(d sub 2) pc where (d sub 2) is the distance to CTB 80 in 2 kpc, and a total H I mass of 1200 (d sup 2, sub 2) solar masses. With its measured kinematic and dynamical properties, CTB 80 provides a 'Rosetta Stone' for studies of old SNRs.

PB91-175026 Not available NTIS
National Inst. of Standards and Technology (NML),
Boulder, CO. Quantum Physics Div.
Ground-Truth Observations of Stellar Surface
Structure from the Lunar Surface.
Final rept.

Final rept. J. L. Linsky. 1990, 10p Grant NAG5-82

Sponsored by National Aeronautics and Space Admin-

istration, Washington, DC. Pub. in Proceedings of NASA Workshop on Astrophysics from the Moon, Annapolis, MD., February 1990, p168-177.

Keywords: \*Stellar activity, \*Lunar observatories, Lunar surface, Stellar chromospheres, Starspots, Granulation, Convection, Interferometry, Reprints.

Using increasingly sophisticated observing strategies, astronomers have begun to observe brightness inhomogeneities on the surfaces of stars indicative of star-spots, active regions, and chemically-anomalous patches with size scales far smaller than the diffraction limits of the present generation of telescopes. While tantalizing, these first glimpses of stellar surface struc-tures are very crude and not unique. Modest-sized op-tical and ultraviolet interferometers located on the lunar surface could resolve these surface structures on nearby, bright stars to provide 'ground truth' to the present crude images and to extend the studies to much smaller and physically interesting scales. An intermediate scale optical/ultraviolet interferometer on the lunar surface with 0.001 to 0.0001 arcsecond angular resolution would provide unique and spectacular results concerning stellar surface structures. The intermediate scale interferometer could be a very useful device for learning how to build larger interferometers that could address more difficult questions.

PB91-175034 Not available NTIS
National Inst. of Standards and Technology (NML),
Boulder, CO. Quantum Physics Div.
Some Concluding Thoughts for Cool Stars VI.

Final rept. J. L. Linsky. 1989, 4p Grant NAG5-82

Sponsored by National Aeronautics and Space Admin-

istration, Washington, DC.
Pub. in Proceedings of Cambridge Workshop on Cool
Stars, Stellar Systems, and the Sun (6th), Seattle, WA.,
September 12-14, 1989, p500-503.

Keywords: \*Cool stars, Stellar chromospheres, Stellar coronae, Stellar winds, Late stars, Meetings, Reprints.

In the Workshop summary the author highlights some of the major trends in the field of cool stars research and calls attention to some of the important unanswered questions that the author hopes will become the scientific highlights of the next Workshop.

100,031 PB91-175042

Not available NTIS

National Inst. of Standards and Technology (NML), Boulder, CO. Quantum Physics Div. Extension of the Class of Magnetic B Star Nonther-

mal Radio Sources.

Final rept. J. L. Linsky, S. A. Drake, and T. S. Bastian. 1990, 4p. Grant NAGW-1716

Sponsored by National Aeronautics and Space Admin-

istration, Washington, DC.
Pub. in Proceedings of Cambridge Workshop on Cool
Stars, Stellar Systems, and the Sun (6th), Seattle, WA., September 12-14, 1989, p189-192 1990.

Keywords: \*Radio sources(Astronomy), \*Magnetic stars, \*B stars, Reprints.

The authors have extended the initial Drake et al (1987) survey in 3 subsequent VLA runs, and have not detected a total of 15 sources at 6 cm. Of these stars 3 are also detected at 2 cm, 3 at 3.6 cm, and 5 at 20 cm. The authors have found no additional early-B Hestrong stars, but have detected 10 new stars with spectral types B5-AO that have measured magnetic fields and are generally He-weak and Si-strong. The authors have not yet detected any classical Ap stars despite a number of attempts.

PB91-200873 Not available NTIS

Not available 1415
National Inst. of Standards and Technology (NML),
Boulder, CO. Quantum Physics Div.
Energy Distributions of Symbiotic Novae.

G. L. Bryan, and S. Kwok. 1991, 9p Pub. in Astrophysical Jnl. 368, p252-260, 10 Feb 91.

Keywords: \*Symbiotic stars, \*Noval, Infrared astronomy satellite, Infrared spectra, Ultraviolet spectra, Stellar envelopes, IUE, Reprints.

The IRAS low-resolution spectra of three recent symbiotic novae (HM Sge. V1016 Cyg, and RR Tel) are fitted with a dust continuum radiative transfer model. It was found that the dust shells are detached from the photosphere and that the sizes of the inner radii are correlated with times since outburst. An analysis of the IUE spectra of HM Sge at different epochs suggests that the strength of the 2200 A feature is decreasing with time and the grains responsible for the feature are probably formed in the white dwarf ejecta. A complete accounting of the entire energy budget from radio to X-ray shows that most of the energy is emitted by the cool component in the infrared, and a significant fraction of the flux of the hot component is escaping in the far-ultraviolet. The density-bounded nature of the circumstellar gas nebulae could be the result of a bipolar geometry of the nebulae. Unlike classical novae, the optical outburst of symbiotic novae is due to the ioniza-tion of the preexisting envelope of the cool component and is not the result of a sudden ejection by the hot component.

Not available NTIS PB91-202861 National Inst. of Standards and Technology (NML), Boulder, CO. Quantum Physics Div. **Evolution of Infrared Carbon Stars.** Final rept.

S. J. Chan, and S. Kwok. 1990, 15p Sponsored by Natural Sciences and Engineering Research Council of Canada, Ottawa (Ontario).

Pub. in Astronomy and Astrophysics 237, p354-368

Keywords: \*Carbon stars, \*Stellar evolution, Infrared astronomy satellite, Stellar mass ejection, Stellar envelopes, Infrared stars, Late stars, Reprints, Mass

The Infrared Astronomical Satellite (IRAS) survey has shown that carbon stars which were discovered by optical surveys and those identified as such because of their SiC dust features have very different infrared colors. The former is visually bright and has large excesses in 60 micrometers while the latter (which will be referred to as infrared carbon stars) have blackbody-like energy distributions. In the present paper, the au-thors present model calculations on the evolution from visual carbon stars to infrared carbon stars. The authors have selected a sample of 472 infrared carbon stars from the IRAS Low Resolution Spectra (LRS) Atlas after rejecting mis-classified objects. A new opacity function for the SiC grain is derived from the LRS of the brightest sources in this sample. The energy distributions of about 150 IRAS infrared carbon stars are fitted with a radiative transfer model. The

evolution of infrared carbon stars can be understood by a continuous increase in mass loss rate on the asymptotic giant branch (AGB).

# **ATMOSPHERIC** SCIENCES

#### Physical Meteorology

100.034

Not available NTIS PB91-189340 National Inst. of Standards and Technology (NML), Gaithersburg, MD. Gas and Particulate Science Div.

Reference NO2 Calibration System for Ground-Based Intercomparisons during NASA's GTE/CITE

Final rept.

A. Fried, L. Nunnermacker, B. Cadoff, R. Sams, N. Yates, W. Dorko, R. Dickerson, and E. Winstead.

Pub. in Jnl. of Geophysical Research - Atmospheres 95, nD7 p139-146 1990.

Keywords: \*Nitrogen dioxide, Atmospheric composition, Calibration, Reprints, \*Reference materials, Global Tropospheric Experiment, Intercomparison.

An NO2 calibration system, based upon a permeation tube and a two stage dynamic dilution system, was designed, constructed, and characterized at the National Bureau of Standards. The calibration system described was employed as the reference standard in NASA's Global Tropospheric Experiment/CITE-II mission in August of 1986, and was capable of accurately delivering known NO2 concentrations in the 0.4 to 200 ppby concentration range with a total uncertainty around 10%. Extensive laboratory tests were carried out based upon gravimetry, chemiluminescence detection, and tunable diode laser absorption spectroscopy, to characterize both the system performance and the permeation emission rate. Upon completion of these tests, the calibration system was mounted on board NASA's research aircraft at both the Wallops Island and Ames research facilities. Known NO2 concentrations in the 0.4 to 1 ppbv range were delivered to four different NO2 detectors in a double blind intercomparison.

100,035

PB91-236646 Not available NTIS National Inst. of Standards and Technology (CSTL), Gaithersburg, MD. Organic Analytical Research Div. Analysis of Wet Deposition (Acid Rain): Determination of the Major Anionic Constituents by Ion Chromatography.

Final rept.

R. A. Durst, W. Davison, K. Toth, J. E. Rother, M. E. Peden, and B. Griepink. 1991, 9p

Sponsored by International Union of Pure and Applied Chemistry, Oxford (England).

Pub. in Pure and Applied Chemistry 63, n6 p907-915 1991

Keywords: \*Acid rain, \*Deposition, \*Chemical analysis, \*Anions, Air pollution detection, Precipitation(Meteorology), Wet methods, Sampling, Quality assurance, Sample preparation, Comparisons, Reprints, \*Ion chromatography.

For the purposes of the document, only the major anionic constituents of wet deposition, i.e., chloride, sulfate and nitrate, will be considered. The objective of the document is to provide a set of recommended pro-cedures for the collection, handling, and analysis of acid rain samples, and the quality assurance of the resulting data. The use of these procedures should result in greater comparability between laboratories and consequently improved reliability in data interpretation.

# **BEHAVIOR & SOCIETY**

#### Education, Law, & Humanities

100.036 PB91-147744 Not available NTIS National Inst. of Standards and Technology (NCSL), Gaithersburg, MD. Systems and Software Technology

Interactive Courseware Is Leading the Multimedia Movement.

Final rept.

J. Moline. 1990, 5p

Pub. in UNIX Technology Advisor 2, n7 p14-18 Jul 90.

Keywords: \*Computer assisted instruction, \*Training devices, Computer systems programs, Operating systems (Computers), Auxiliary equipment(Computers), Systems engineering, Interactive systems, Reprints, PORTCO(Portable Courseware Project), Multimedia.

The Federal government and other U.S. organizations are developing multimedia training materials for delivery on computer-based interactive training systems. A variety of computers and peripheral devices hosting various operating systems and suites of authoring system software are being used to develop the courseware. The Department of Defense's Portable Courseware Project (PORTCO) is typical of such projects. PORTCO strategy is applicable to all projects. that require an open system environment in which to achieve mission objectives.

Not available NTIS PB91-148114 National Bureau of Standards (NEL), Gaithersburg, MD. Center for Mfg. Engineering.

Agenda for Progress in Technology Education: A Personal View.

Final rept.

D. A. Swyt. 1987, 6p Pub. in Technology Teacher 47, n1 p3-8 Sep/Oct 87.

Keywords: \*Education, \*Technology transfer, Methodology, Training, Reprints, Vocational education

The U.S. as a productive economy and social system is in the midst of a technological transformation that is fundamentally changing how people live and how they earn their livelihoods. This change is straining our educational system, requiring innovation under duress. With technology as both the source of change and the With technology as both the source of change and the remedy for the problems which change entails, the matter of teaching about technology has become a strategic issue. As such, the situation calls for a new agenda for progress in technology education. The paper presents a personal view on the situation and an agenda for change by which technology educators might deal with it. might deal with it.

100.038 Not available NTIS PB91-158725 National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Applied and Computational Mathematics Div.

Engineers' Statistical Literacy Is Key to U.S. Competitiveness. Final rept.

J. T. Fong. 1989, 2p Pub. in ASME News 9, n5 pl and p5 Oct 89.

Keywords: \*Engineering education, \*Statistics, \*Probability theory, Curricula, Mathematics, Experimental design, Data analysis, Stochastic processes, Quality control, Reprints, ABET(Accreditation Board for Engineering and Technology) neering and Technology).

Highlights of a conference entitled 'Statistics and Probability in Engineering Education' are reported. The conference brought together engineering, mathematics, and statistics educators as well as industry and government leaders to discuss the need for incorpo-rating statistical experimental design, data analysis, stochastic processes, probability, quality management technology, and other related areas into the engineering curricula. Two keynote speakers challenged the

educators to reform engineering curricula immediately to improve statistics education, which was judged so inadequate for most engineering colleges as to have resulted in numerous crops of 'statistically illiterate' graduates in the eyes of several industries which employed them. The conference ended with three action items and a resolution to move forward in addressing the critical issues raised.

#### Job Training & Career Development

100,039 PB91-143362 PC A04/MF A01 National Inst. of Standards and Technology (NCTL), Gaithersburg, MD. Office Systems Engineering Group. Multimedia Courseware in an Open Systems Environment: A Federal Strategy.

J. Moline, A. L. Hankinson, and L. A. Welsch. Dec

90, 55p NISTIR-4484

Keywords: \*Computer program portability, \*Computer assisted instruction, \*Training, Interfaces, Standards, Open systems interconnections, \*Interactive systems, National government, Strategy, Computer software, Multimedia, National Institute of Standards and Technical In nology, Off the shelf computer software, Commercial

The Department of Defense (DoD) Portable Courseware Project (PORTCO) is typical of projects worldwide that require standard software interfaces. document articulates the strategy whereby PORTCO leverages the open systems movement and the new realities of information technology. The Federal strategy for multimedia courseware is to facilitate the creation of an environment in which high quality portable courseware is available as commercial off-the-shelf products competitively supplied by vendors. The Request for Architecture déveloped cooperatively by DoD and NIST will generate a portable courseware system architecture incorporating standards which meet users' needs. A computer-based interactive training applications profile must be developed which, along with the system architecture, will provide the basis for identifying needed standards. NIST will then accelerate the development of these standards through established standards forums.

# BIOMEDICAL **TECHNOLOGY & HUMAN FACTORS** ENGINEERING

#### **Biomedical Instrumentation &** Bioengineering

100,040 PB91-148668 Not available NTIS National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Polymers Div.
Setting Reactions and Compressive Strengths of

Calcium Phosphate Cements.

Final rept. Y. Fukase, E. D. Eanes, S. Takagi, L. C. Chow, and W. E. Brown. 1990, 5p

Sponsored by American Dental Association Health Foundation, Chicago, IL.

Pub. in Jnl. of Dental Research 69, n12 p1852-1856

Keywords: \*Calcium phosphates, \*Dental materials, \*Acid bonded reaction cements, Implantation, Setting time, Bones, Compressive strength, Surface chemistry, Chemical analysis, X-ray diffraction, Time dependence, Reprints.

Setting reactions and compressive strengths of a selfhardening calcium phosphate cement (ČPC) were investigated. The CPC consists of tetracalcium phos-

phate (TTCP) and anhydrous dicalcium phosphate (DCPA). The cement specimens were prepared by mixing 0.7 g of the powder (TTCP 72.9 wt% + DCPA 27.1 wt%) with 0.175 mL of the liquid (25 mmol/L H3PO4 and 1.32 mmol/L sodium fluoride). The specimens were removed from the molds at pre-determined time intervals after being mixed, and their compressive ume intervals after being mixed, and their compressive strengths were measured. Immediately afterward, the fractured specimens were rapidly frozen in ethanol (-80 C), lyophilized, and examined by powder x-ray diffraction and scanning electron microscopy (SEM). The results showed that (1) hydroxyapatite was the only reaction product; (2) the reaction was nearly completed within four by during which both the reaction product. within four h, during which both the reaction product and compressive strength increased linearly with time, resulting in a strong correlation between the two; and (3) fully set CPC consisted primarily of small rod-like crystals and some platy crystals.

PB91-150029 Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Chemical Engineering Science Div. PB91-150029 Low-Cost Low-Volume Carrier (Minilab) for Bio-

technology and Fluids Experiments in Low Gravi-

final rept.

J. M. Cassanto, W. Holemans, T. Moller, P. Todd, R. M. Stewart, and Z. R. Korzun. 1990, 15p Sponsored by National Aeronautics and Space Admin-

istration, Washington, DC. Commonwealth of Pennsylvania.

Pub. in Space Commercialization: Platforms and Processing, v127 p199-213 1990.

Keywords: \*Reduced gravity, \*Automatic control, \*Space laboratories, \*Remote control, Membranes, Interfaces, Interfacial tension, Space flight, Experimental design, Biotechnology, Research projects, Polymeric films, Miniaturization, Reprints.

Research opportunities in biotechnology and fluid technology under conditions of microgravity can be made available to research workers from developing countries through relevant research projects and lowcost access to microgravity environments. Examples of such projects include polymeric film formation, purification methodology, liquid-liquid diffusion, and growth of organic and protein crystals. An example of a low-cost research device is the Materials Dispersion Apparatus (MDA) which can be used to conduct important low-volume experiments in an automated fashion wherever pairs, or groups of pairs, of liquids must inter-act. The MDA is designed to be compatible with sever-al carriers: shuttle middeck lockers, Get-Away Special canisters, Hitchhiker, Lifesat, recoverable re-entry vehicles, low-gravity aircraft flights, and sounding rockets. The MDA consists of a pair of sliding blocks, in which wells in one block move into contact with wells in the other block under electronic command. Requirements for power, including temperature control, are minimal. Experiments related to biotechnology have minimal. Experiments related to biotechnology have been designed for a single flight of the MDA in which the carrier will be a sounding rocket that provides approximately 6 min of low gravity. Examples of experiments to be conducted include the nucleation of organic crystals in aqueous solution, behavior of immiscible aqueous solutions, solid-liquid surface phenomena at high surface-tension gradients, and the formation of this polymeric membranes. tion of thin polymeric membranes.

100 042 Not available NTIS PB91-158493 National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Polymers Div.

Visco-Elastic Deformation of Dental Porcelain and

Porcelain-Metal Compatibility.

K. Asaoka, and J. A. Tesk. 1991, 6p Sponsored by National Inst. of Dental Research, Be-

Pub. in Dental Material 7, n1 p30-35 Jan 91.

Keywords: \*Dental materials, Heat treatment, Firing, Dissimilar materials bonding, Metals, Porcelain, Stress analysis, Viscoelasticity, Computerized simulation, Deformation, Thermal expansion, Reprints.

A computer simulation using a visco-elastic stress analysis was conducted to clarify the effect of the heating rate on deformation temperature of dental porcelain during firing. In the simulation, the following temperature-dependent factors were incorporated: elastic modulus, viscosity, and coefficient of thermal expansion. Thermal expansion curves of porcelain with an

# **BIOMEDICAL TECHNOLOGY & HUMAN FACTORS ENGINEERING**

# Biomedical Instrumentation & Bioengineering

applied load at various heating rates were computed. The results suggest that the temperature where the incompatibility stress develops in the porcelain-fused-tometal strips during cooling can be estimated closely from the deformation point of the heating curve of the porcelain with an applied stress of about 1.2 - 3.1 MPa.

PB91-158691 Not available NTIS Not available NTS National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Polymers Div. Effect of Catalyst Structure on the Synthesis of a

Dental Restorative Monomer.

Final rept. M. Farahani, A. D. Johnston, and R. L. Bowen. 1991,

Sponsored by American Dental Association Health Foundation, Chicago, IL. Pub. in Jnl. of Dental Research 70, n1 p67-71 Jan 91.

Keywords: \*Acid bonded reaction cements, \*Dental materials, Molecular isomerism, Synthesis(Chemistry), Catalysts, Amines, Ethylamine, Hexamethylenetetramine, Pyromellitic acid, Reprints, Pyromellitic dianhydride, Diisopropylethyamine.

The addition product of 2-hydroxyethyl methacrylate (HEMA) and pyromellitic dianhydride (PMDA), known as PMDM, is a mixture of two structural isomers. The para PMDM isomer--currently used in mediating adhesive bonding of restorative materials to hard tooth issues--is a crystalline solid. The meta isomer is a liquid. In the synthesis of PMDM, the para isomer, which can be purified by crystallization, is usually present to the extent of only 50% of the product mixture. The effect of the amine catalyst structure was studied relative to its role in increasing the yield of the para isomer, either by a reduction in the amount of the meta isomer or by an increase in the extent of overall reaction. The chemical structure of the amine catalyst had an important role in the synthesis of PMDM and influenced the ratio of the isomers. Among aliphatic amines, especially noteworthy as catalysts that gave excellent yields of the para isomer in high purity were N, N-di-isopropyl-ethylamine and hexametylenetetra-

100,044 PB91-159210 Not available NTIS National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Polymers Div.

Dental Biomaterials and Engineering Frontiers for the 90's. Final rept.

J. A. Tesk. 1990, 2p

Pub. in Proceedings of the International Kyoto Symposium on Biomedical Engineering (3rd), Kyoto, Japan, November 20-21, 1990, p14-15.

Keywords: \*Dental materials, \*Biotechnology, Reprints, \*Biomedical engineering.

Some areas of dental materials and engineering which should receive increased attention in the 1990's are discussed.

Not available NTIS PB91-174458 National Inst. of Standards and Technology (IMSE), Gaithersburg, MD. Polymers Div.

Glass-Ceramic Inserts Anticipated for 'Megafilled' Composite Restorations.

Final rept. R. L. Bowen, F. C. Eichmiller, and W. A. Marjenhoff. 1991, 3p

Sponsored by American Dental Association Health Foundation, Chicago, IL.
Pub. in Jnl. of the American Dental Association 122,

p71, 73, and 75, Mar 91.

Keywords: \*Dental materials, \*Composite materials, Ceramics, Glass, Inserts, Color, Dimensional stability, Physical properties, Reprints.

Further improvement in the physical properties of directly placed composites is expected with the introduction of preformed, tooth-colored glass-ceramic inserts for Class I, II and III megafilled restorations. Less microleakage is associated with restorations containing inserts. Inserts are also expected to increase the stiffness, strength and durability of composite restorations, promote dimensional stability of the remaining tooth crown during hardening and function, and offer the esthetic advantage of having inherent tooth shades. It is anticipated that the first commercial inserts kits (perhaps available within the year) will be

comprised of three to four standardized shapes in three to four sizes, in the most utilized tooth shades. The additional time required for placement and finishing of inserts by dentists is not expected to be more than two or three minutes. Inserts are expected to add only about a dollar each to the cost of materials used in a composite restoration and should not, therefore, categorically increase current fee structures.

PB91-174490 Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Automated Production Technology Div.

Correction for Converting 2-CM(3)-Coupler Re-

sponses to Insertion Responses for Custom in-the-Ear Non-Directional Hearing Aids. Final rept.

E. D. Burnett, and L. B. Beck. 1987, 6p Pub. in Ear Hear 8, p89S-94S Oct 87.

Keywords: \*Hearing aids, Fourier analysis, Frequency response, Measurement, Responses, Correction, Comparison, Reprints.

A correction for custom in-the-ear non-directional hearing aids is obtained for converting a frequency response obtained using a 2-cm cubed coupler to an insertion response, approximating that measured using a manikin and ear simulator. The results are compared to those of a previous published study. The methods used for obtaining the responses make use of a signal analyzer with discrete Fourier transform capabilities.

PB91-189555 Not available NTIS National Inst. of Standards and Technology (IMSE), Gaithersburg, MD. Polymers Div. Protective Coatings for Tooth Crowns.

A. D. Johnston, and R. L. Bowen. 1991, 3p Sponsored by American Dental Association Health Foundation, Chicago, IL.

Pub. in Jnl. of the American Dental Association 122, p49-51 Apr 91.

Keywords: \*Dental materials. \*Dental caries. \*Polymeric films, \*Protective coatings, Surface chemistry, Enamels, Hydrophylic polymers, Reprints.

The application (and occasional renewal) of invisible polymeric films to entire tooth crown surfaces may someday be an effective means of caries prevention for patients of all ages.

100,048

PB91-194654 Not available NTIS National Inst. of Standards and Technology (IMSE), Gaithersburg, MD. Polymers Div. Filler Systems Based on Calcium Metaphosphates.

J. M. Antonucci, B. O. Fowler, and S. Venz. 1991, 6p Sponsored by National Inst. of Dental Research, Be-

Pub. in Dental Materials 7, p124-129 Apr 91.

Keywords: \*Dental materials, \*Calcium phosphates, \*Dental caries, \*Fillers, \*Inorganic polymers, Teeth, Chemical radiation effects, Ultraviolet radiation, Refractivity, Crack arrest, Composite materials, Microscopy, Reprints.

Calcium metaphosphates (CMP's) -- a unique class of phosphate minerals possessing polymeric structures, (Ca(PO3)2)n, and having refractive indices of 1.54-1.59 are optically compatible with resins such as BISGMA. Several types of CMP's were prepared and evaluated for their potential as fillers for visible-light-activated (VLA) dental composites. The vitreous (V) and beta-crystalline forms of CMP were prepared by controlled thermolysis of monocalcium phosphate monohydrate. Hybrid fillers were also prepared by thermal methods. Fillers, characterized by IR spectroscopy and optical microscopy, were prepared in several size ranges (e.g., 1-100 micrometers). Beta-CMP composites were more moisture-resistant, had higher diametral tensile strengths (from 12 to 33 MPa), and showed a tendency to arrest brittle fracture. These novel fillers have potential uses in resin-based materials such as dental composites, cements, and adhesives.

100.049 PB91-202879 Not available NTIS National Inst. of Standards and Technology (IMSE), Gaithersburg, MD. Polymers Div.

Self-Setting Calcium Phosphate Cements.

Final rept. L. C. Chow, S. Takagi, P. D. Costantino, and C. D. Friedman. 1991, 22p
Sponsored by American Dental Association Health
Foundation, Chicago, IL.
Pub. in Materials Research Society Symposium Pro-

ceedings, v179 p3-24 1991.

Keywords: \*Calcium phosphates, \*Dental materials, \*Medical supplies, \*Cements, Binary system(Materials), Phosphoric acid, Aqueous solutions, Mixtures, Apatites, Hydroxy compounds, Biocompatibility, Hardness, Reprints, Self-setting.

A mixture of tetracalcium phosphate and dicalcium phosphate, when mixed with a dilute phosphoric acid or other aqueous solutions, will harden like a cementproducing hydroxyapatite as the final product. The latter is the principal mineral component of hard tissue. The chemistry, physical properties, and biocompatibility of the calcium phosphate cement are discussed. The setting property, combined with high biocompatibility, makes calcium phosphate cements useful in many applications in dentistry and medicine.

100,050

PB91-204081 Not available NTIS National Bureau of Standards (IMSE), Gaithersburg, MD. Polymers Div.

Microstructure and Elastic Properties of Dental Resin and Resin-Based Glass-Reinforced Composites: XRD, SEM and Ultrasonic Methods. Final rept.

S. Singh, J. L. Katz, J. Antonucci, R. W. Penn, and J. A. Tesk. 1988, 6p
Pub. in Materials Research Society Symposium Pro-

ceedings, v110 p599-604 1988.

Keywords: \*Resin matrix composites, \*Fiber composites, \*Fiberglass, \*Dental materials, \*Dental caries, Elastic properties, Microstructure, X-ray diffraction, Scanning tunneling microscopy, Mechanical properties, Nondestructive tests, Ultrasonic tests, Amorphous materials, Poisson ratio, Young modulus, Silanes, Velocity, Density, Polymers, Reprints, Energy dispersive spectrometry.

The load-bearing ability of dental restorative materials under cyclic high-stress applications depends upon mechanical properties established by the composition and microstructure. The microstructure and the elastic properties of neat resin and two resin-based glass-reinforced composites have been studied. The microstructure of these materials has been examined using xray diffractometry (XRD), scanning electron microsco-(SEM) including energy dispersive spectrometry py (SEM) including energy dispersive specializing (EDS). The elastic properties, i.e., Young's, shear and bulk moduli and Poisson's ratio were determined from ultrasonic velocities and densities. The ultrasonic velocities were measured using a pulse-through transmission method; density was measured using a buoyant force method. These studies showed that: (1) these materials have amorphous structures; (2) these materials have Young's moduli of the order of 20 GPa, and (3) the silane coupling agent apparently did not significantly affect the elastic properties of these resinbased composites.

100.051

PB91-204149 Not available NTIS National Bureau of Standards (IMSE), Gaithersburg, MD. Polymers Div. Dental Composite Resins: An Update.

Final rept. S. Venz. 1987, 2p Pub. in Modern Dentalab 5, n4 p27-28 Jun/Jul 87.

Keywords: \*Dental materials, \*Dental caries, \*Resin matrix composites, PMMA, Radiation curing, Visible radiation, Methacrylates, Surface treatments, Inorganic compounds, Polymers, Plastics, Reprints, Self-curing.

Since the introduction of self-curing dental restorative resins in the 1940s, numerous modifications have been introduced to enhance the performance of resinbased restorations in the oral cavity. Major developments leading to current dental composite resins are the use of di- or polyfunctional methacrylates instead of the monofunctional methyl methacrylate, the incor-poration of surface treated inorganic fillers instead of poly-(methylmethacrylate) powder and the introduc-tion of visible light curing, single component materials instead of two part chemical curing systems.

## BIOMEDICAL TECHNOLOGY & HUMAN FACTORS ENGINEERING

#### Biomedical Instrumentation & Bioengineering

100,052 PB91-236539 Not available NTIS National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Polymers Div.

Development of an Adhesive System for Bonding

to Hard Tooth Tissues.

Final rept.

R. L. Bowen, and W. A. Marjenhoff. 1991, 5p.

Sponsored by American Dental Association Health Foundation, Chicago, IL.

Pub. in Jnl. of Esthetic Dentistry 3, n3 p86-90 May/Jun

Keywords: \*Acid bonded reaction cements, \*Adhesives, \*Dental materials, Composite materials, Enamels, Dentin, Teeth, Reviews, Inorganic silicates, Resins, Aqueous solutions, Synthesis(Chemistry), Re-

The development of an adhesion system for bonding dental composites to dentin and enamel is reviewed. Building on findings concerning adhesion to enamel, R. L. Bowen and colleagues at the Paffenbarger Re-H. L. Bowen and colleagues at the Pattenbarger Research Center, National Institute of Standards and Technology, began addressing and solving problems associated with (1) silicate cements and unfilled resins; (2) bonding in an aqueous environment; and (3) the development of an adhesion system for both dentin and enamel that could withstand various stresses. Although commercial products based on the adhesion system are currently available in the dental materials marketials environmentation continues for materials marketplace, experimentation continues, focusing on the synthesis of potentially better component analogs, the optimization of the individual components, and on improved storage stability and ease of synthesis.

PB91-237735 Not available NTIS PB91-237735
National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Polymers Div.
Dentin-Bonding Molar Efficiency Using N-Phenylglycine, N-Phenyl-beta-Alanine, or N-Methyl-N-

lycine, N-Phenyl-beta-Alanine, or Phenylglycine.

Prenyigyone.
Final rept.
R. E. Webb, and A. D. Johnston. 1991, 4p
Sponsored by American Dental Association Health
Foundation, Chicago, IL.
Pub. in Jnl. of Dental Research 70, n3 p211-214 Mar

Keywords: \*Amino acids, \*Bonding strength, \*Dentin, \*Acid bonded reaction cements, \*Adhesives, Phenylalanine, Glycine, Methyl compounds, Teeth, Nitrogen organic compounds, Alanines, Oxalates, Iron complexes, Dental materials, Reprints, Molar efficiency

Three structurally related substituted amino acids (Ncompounds) were studied in a three-step dentin-bonding protocol. In the second step, the amount of the N-compound--either N-phenylglycine (NPG), N-methyl-N-phenylglycine (NMNPG), or N-phenyl-beta-alanine N-phenylglycine (NMNPG), or N-phenyl-beta-alanine (NPBA)--was varied in acetone from 0 mol/L through 0.5 mol/L in A+0.001 mol/L for NPG and NMNPG, average bond strength values were 7.4 + or -2.2 and 10.5 + or -2.7 MPa. The highest bond strength value for NMNPG was at 0.01 mol/L, with 13.2 + or -4.0 MPa. The highest value for NPG was at 0.1 mol/L, with a value of 11.8 + or -2.5 MPa. The average bond strength for NPBA did not differ from zero across the entire range of concentrations. Molar efficiency was defined as the bond strength per mole of these applied defined as the bond strength per mole of these applied N-compounds. For the two N-compounds that did provide adhesion to dentin, NPG and NMNPG, the average bond strengths rose, peaked, and fell as the amounts of applied N-compound were increased. The molar efficiency dropped off as the concentration of applied N-compound rose.

#### **Prosthetics & Mechanical Organs**

PB91-194761 Not available NTIS National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Polymers Div. Metal-Polysiloxane Shields for Radiation Therapy of Maxillo-Facial Tumors.

Final rept.

M. Farahani, F. C. Eichmiller, and W. L. McLaughlin. 1991. 6p.

Sponsored by American Dental Association Health Foundation, Chicago, IL.

Pub. in Medical Physics 18, n2 p273-278 Mar/Apr 91.

Keywords: \*Radiotherapy, \*Radiation therapy, \*Shielding, \*Gamma rays, Tissues, Dosimetry, Particulate composites, Oral diseases, Maxillary neoplasms, Face(Anatomy), Neck(Anatomy), Prosthetic devices, Mouth neoplasms, Molding materials, Cobalt 60, Synthesis alexans. thetic elastomers, Resin matrix composites, Siloxanes, Binary alloys, Vinyl compounds, Silver alloys, Copper alloys, Tin alloys, Antimony alloys, Reprints.

In the treatment of some head and neck lesions with high-intensity radiation (teletherapy), an essential pro-cedure is the application of an individually customized shielding appliance, which is designed, modeled, and formed into a working extra- or intraoral stent for the purpose of sparing healthy tissues. The present state of the art is slow and technique intensive, which can add to patient discomfort and inconvenience during molding and fabrication. A new formulation is described, which offers speed and ease of forming a moldable composite stent especially for intraoral use. Tests using collimated gamma-ray beams from a (60)Co teletherapy unit were made in order to measure the dose distribution near interfaces of tissue-simulat-ing polymer and the composite stent material with and without mixtures of metals (Ag-Cu and Sn-Sb). The results show that quickly formed composites made of a flexible resin with high concentrations of powdered spherical metal alloys provide effective custom-de-signed shielding, and, with a thin overlayer of the resin without metal, a dimished back-scattered radiation dose to normal tissues. An example of a successful formulation is a mixture of 90% by weight Ag-Cu alloy powder in a vinyl polysiloxane resin. The material is a moldable putty which, upon polymerization, forms a rigid elastomeric material, providing a half-value layer of approximately 2.5 to 2.8 cm for a gamma-ray beam from a (60)Co source.

PB91-194787 Not available NTIS National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Metallurgy Div. Corrosion Principles in Dental Implantology.

Final rept. A. C. Fraker, and F. Eichmiller. 1990, 10p Pub. in Clark's Clinical Dentistry, Chapter 50, v1 p1-10

Keywords: \*Dental materials, \*Titanium alloys, \*Implants, \*Corrosion, \*Prosthetic devices, Dissimilar materials bonding, Performance prediction, Apatites, Solid-solid interfaces, Tissues, Surface chemistry, Hydroxy compounds, Reprints.

Corrosion processes that could occur with dental implants and some guidelines for predicting the corrosion behavior of common prosthetic alloys are given. Interactions between dissimilar materials within the prosthetic device can result in corrosion, and this is discussed. The titanium implant will be covered with a surface oxide or with an applied layer of hydroxyapatite. The implant/tissue interface is described and discussed.

100.056 PB92-117407 Not available NTIS National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Polymers Div. Comparative Study of Bovine Pericardium Mineralization: A Basic and Practical Approach.

Final rept.

B. B. Tomazic, C. Siew, and W. E. Brown. 1991, 11p Sponsored by American Dental Association Health Foundation, Chicago, IL. Pub. in Cells and Materials 1, n3 p231-241 1991.

Keywords: \*Mineralization, \*Pericardium, \*Heart valve prosthesis, Cattle, Comparison, In vivo analysis, In vitro analysis, Calcinosis, Histology, Rats, Humans,

The biomineralization of bovine pericardium (BP) heart valve bioprostheses was investigated by simulation of the process under in vitro and in vivo conditions. The nature and composition of calcific deposits that formed in human heart valve bioprostheses were compared with the mineral formed on BP discs immersed in a calcifying medium or subcutaneously implanted into Sprague-Dawley rats. The early stage of experimental biomineralization in vitro took place on the surface only, while in vivo deposition appeared to be intrinsic, as documented by histological cross sections. Combined information from in vitro, in vivo and bioprosthetic mineralization supports the concept that octacalcium phosphate is a precursor that transforms into bioapatite and is implicated in the calcification of bioprosthetic heart valves.

# **BUILDING INDUSTRY TECHNOLOGY**

#### **Architectural Design & Environmental** Engineering

100,057

PB91-147082 Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Building Physics Div.
Calibration Procedures for Infrared Imaging Sys-

tems for Building Diagnostics.

Final rept.
Y. M. Chang, and R. A. Grot. 1986, 8p
Sponsored by Department of Energy, Washington, DC.
Pub. in Proceedings of International Symposium on
Temperature Measurement in Industry and Science,
Beijing, China, April 16-19, 1986, p277-284.

Keywords: \*Calibration, \*Infrared equipment, \*Temperature measuring instruments, \*Heat loss, \*Buildings, Temperature measurement, Frequencies, Inspection, Heat transmission, Energy conservation, Standards, Reprints.

The paper describes laboratory measurements for the evaluation of infrared imaging systems commonly used for building inspections. The infrared imaging systems were evaluated at various background temperatures ranging from -20 to 25C. The tests performed on each infrared imaging system were the determination of the minimum resolvable temperature difference (MRTD) at spatial frequencies ranging from 0.03 to 0.25 cy/mrad and calibration curves of the measured radiosity (isotherm level) versus the equivalent blackbody temperature of the target. The results of the MRTD tests are compared with the theory used in the ASHRAE Standard 101-83. It is shown that the theory accurately predicts the temperature dependence of the MRTD curves only for one infrared imaging system operating in the 2 to 5 micrometer range. For infrared imaging systems in the 8 to 12 micrometer range, the MRTD increases much faster as the object temperature decreases than predicted by the theory. It is also shown that the calibration curves of the two tested infrared imaging systems operating in the 8 to 12 micrometer range have a strong temperature dependence.

100,058 PB91-147140 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Building Environment Div. Second-Level Post-Occupancy Evaluation Analy-

Final rept. B. L. Collins, W. Fisher, G. Gillette, and R. W.

Marans. 1990, 24p See also DE89014520. Pub. in Jnl. of the Illuminating Engineering Society, p21-44 1990.

Keywords: \*Lighting systems, \*Office buildings, \*Comfort, Daylighting, Evaluation, Illuminance, Design, Environmental engineering, Illuminating, Interior lighting, Brightness, Reprints.

Post-occupancy evaluations (POE) have been used by Post-occupancy evaluations (POE) have been used by a number of researchers as a tool for documenting, evaluating, and improving environmental conditions in offices. In a project sponsored by the US Department of Energy and the New York State Energy Research and Development Authority during 1984-1986 POE data were collected on lighting power densities, photometric levels, and user attitudes for 912 workstations in 13 office buildings that contained lighting systems in 13 office buildings that contained lighting systems somewhat typical of current lighting practice. The purpose of the present evaluation is to examine the relationships between individual lighting system type and these data.

## Architectural Design & Environmental Engineering

PB91-147561 Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Building Physics Div. Design Heat Loss Factors for Basement and Slab

Floors.

Final rept.

Philatrick.
T. Kusuda, and J. W. Bean. 1985, 21p
Pub. in Thermal Insulation: Materials and Systems,
ASTM ATP 922, p132-152 1985.

Keywords: \*Heat loss, \*Basements, \*Floors, Design criteria, Thermal insulation, Thermal analysis, Buildings, Concrete slabs, Walls, Slabs on ground construction, Energy conservation, Reprints.

The heat loss factors for selected types of earth conrate loss factors for selected types of earth con-tact surfaces, such as basement walls and floors and slab-on-grade floors, are presented to supplement data in the ASHRAE Handbook of Fundamentals for estimating the building design heat loss. The perimeter heat loss factors are derived from the procedure developed by Mitalas and from monthly normal tempera-ture cycles of many localities in the United States. Except for those for cities in California, the heat loss factors are found to be a relatively well-defined function of degree-days and remain constant for degree-days beyond 3000 (engineering units). The heat loss factors show that the most effective way to reduce the earth contact surface heat loss is to insulate the inside corners of wall/floor joints. The insulation installed below the floor slab is found to be the least effective as long as the wall foundation is left uninsulated.

100,060 PB91-147876 Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Building Physics Div.

Ventilation System Performance Evaluation Using Tracer Gas Techniques.

Final rept.

A. K. Persily, and R. A. Grot. 1985, 17p Sponsored by Department of Energy, Washington, DC. Pub. in Proceedings of AIC Conference (6th) Ventila-tion Strategies and Measurement Techniques, Netherlands, September 16-19, 1985, p26.1-26.16.

Keywords: \*Indoor air pollution, \*Ventilation, \*Tracers, \*Measurement, Performance evaluation, Air quality, Environmental engineering, Leakage, Air flow, Buildings, HVAS systems, Reprints.

Based on current concerns regarding indoor air quality and energy use, there is a need for in situ techniques for evaluating buildings' infiltration and ventilation characteristics. The U.S. National Bureau of Standards has developed and employed equipment and tech-niques for such evaluation. The measurement of whole building leakage and ventilation rates has been reported on previously. Additional procedures are presented here for a more complete evaluation of the ventilation system operation and the distribution of air within the building. The measurements reveal both the amount of outside air infiltrating through the envelope and the amount of intentional intake through the air handlers. Tracer gas techniques to study the uniformity of air distribution throughout a building are also discussed. These in situ evaluation techniques are described and results from their application are presented.

100,061 Not available NTIS PB91-158535 National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Building Environment Div. Conference Coverage: Papers Presentations Shine.

Final rept.

Pub. in Lighting Design and Application, p21-23 Oct

Keywords: \*Illuminating, Energy conservation, Lamps, Computer graphics, US NBS, Meetings, Reprints, Baltimore(Maryland).

The technical highlights from the recent IESNA Conference in Baltimore, MD are summarized in some detail. At the session 48 papers on lighting research, detail. At the session 48 papers on lighting research, technology, design and application were presented. Topics discussed included light sources and conservation issues for displays; efficiency standards for lamps; daylight measurement and modeling; lamp performance including fluorescent, incandescent, metal halide, high pressure sodium, and special sources; tunnel and roadway lighting; measurement and con-

trols; modeling and lighting geometry; calculations; visibility and visual performance; computer graphics; and VDT's. Issues relating to energy conservation, such as efficiency standards, daylighting, and new lamp technology generated considerable attention, as did papers on lighting and conservation as well as computer graphics as a design tool.

100.062

PB91-159079 Not available NTIS National Bureau of Standards (NEL), Gaithersburg,

MD. Building Equipment Div.

Prototype Expert System for Diagnosing Moisture

Problems in Houses.

Final rept.

Pub. in Proceedings of BTECC Symposium on Air Infil-tration, Ventilation, and Moisture Transfer, Fort Worth, TX., December 1986, 10p.

Keywords: \*Expert systems, \*Moisture content, \*Residential buildings, \*HVAC systems, Ventilation, Protoypes, Air flow, Moisture, Indoor air quality, Comfort, Heat loss, Reprints.

A knowledge based expert system is under development to assist in the identification and diagnosis of air leakage problems in residential buildings. The expert system is intended for use by home energy auditors who are familiar with house construction and building performance issues, but do not have the expertise necessary to deal effectively with the wide variety of circumstances encountered in houses. The system development is beginning with a prototype to diagnose moisture-related problems. This prototype is the first step in the development of the more comprehensive expert system that will deal with air leakage problems associated with indoor air quality, thermal comfort, and heat loss and gain. In the paper the moisture-diagnosis prototype is described and discussed. This prototype system requires the user to describe the symptoms of the existing moisture problems and provide information on house characteristics. Based on additional information on the symptoms and the house, this interactive program produces a list of probable causes and recommendations for remedial action. In addition to describing the current prototype system, the paper also discusses the results of an evaluation of the system based on its use by human experts in the field of residential building moisture. This evaluation, along with insights obtained through the efforts of the system's developers, has led to several proposed improvements of the prototype.

100,063

PB91-159293 Not available NTIS Mational Bureau of Standards (NEL), Gaithersburg, MD. Center for Building Technology.

Al: Does It Have a Place in Building Simulation.

Pub. in Proceedings of Building Energy Simulation Conference, Seattle, WA., August 21, 1985, p169-174.

Keywords: \*Artificial intelligence, \*Buildings, Designs, Expert systems, Simulation, Decision making, Architecture, Civil engineering, Design criteria, Construction, Reprints.

Artificial intelligence (AI) technologies and simulation technologies can be combined to support excellent decisions throughout the whole building process. Al technologies are briefly reviewed. Simulation is generalized as a means to predict prototype performance whether in the building process or in the response of the building in use to its natural and man-made environments. Al can assist the decision maker in selecting the simulation scheme, detailing and conducting the simulation, and assessing the validity and meaning of the results of simulation. Simulation can assist the knowledge engineer in the formulation of knowledge bases to guide in decision making for various building problems. Al and simulation technologies are identified as natural and powerful partners for the guidance of decision makers in all phases of the building process. Substantial research, development and education will be required to realize the potential of these technologies to increase the usefulness, safety and economy of buildings.

100,064 PB91-167155 PC 403/MF 401 National Inst. of Standards and Technology, Gaithersburg, MD.

ZIP: The ZIP-Code Insulation Program, Version 2.0. Economic Insulation Levels for New and Existing Houses by Three-Digit Zip Code. Users' Guide and

Reference Manual (Revised Edition).
S. R. Petersen. Jan 91, 36p NISTIR-88/3801-1
See also PB89-159446 and PB89-151765. Sponsored by Department of Energy, Washington, DC. Building

Keywords: \*Residential buildings, \*Thermal insulation, \*Economic analysis, Engineering costs, Climate, Prices, Energy conservation, Life cycle costs, Heating, Cooling, Construction, User manuals(Computer programs), Zip codes, ZIP computer program.

ZIP 2.0 is a revised and updated version of ZIP, the Zip-Code Insulation Program. ZIP is a computer program developed to support the DoE Insulation Fact Sheet by providing users with customized estimates of economic levels of residential insulation. These estimates can be made for any location in the United States by entering the first three digits of its ZIP code. The program and supporting files are contained on a single 5-1/4 in. diskette for use with microcomputers having an MS-DOS operating system. The revised ZIP program calculates economic levels of insulation for attics, cathedral ceilings, exterior woodframe and masonry walls, floors over unheated areas, slab floors, basement and crawlspace walls, ducts in unconditioned spaces, and water heaters. Climate parameters are contained in a file on the ZIP diskette and are auto-matically retrieved by ZIP code. Regional energy prices and insulation costs are also retrieved from the diskette, but these can be overridden to better reflect local conditions.

100,065

PB91-174607 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Building Environment Div. Refrigerant Charge Effects on Heat Pump Per-

Final rept. G. S. Damasceno, P. A. Domanski, S. Rooke, and V.

G. S. Damascello, P. A. Domanski, S. Hooke, and V. Goldschmidt. 1991, 6p Sponsored by Ranco Controls, Erving, TX. Pub. in ASHRAE (American Society of Heating, Refrigerating and Air-Conditioning Engineers) Transactions, v97 pt1 6p 1991.

Keywords: \*Heat pumps, \*Refrigerants, \*Performance, Mass transfer, Thermodynamic properties, Air conditioners, Mathematical models, Steady state, Residential buildings, Experimental data, Reprints.

The capability of predicting the effects of refrigerant charge on the steady-state performance of a heat pump is addressed. Rather extensive test data for one particular residential air-to-air heat pump are com-pared with the predictions of HPSIM, a computer model with the capability of tracking refrigerant mass distribution within the various components. The need to properly account for parasitic volumes and all internal volumes of the heat pump is underscored.

100,066

PB91-174649 Not available NTIS
National Inst. of Standards and Technology (NEL),
Gaithersburg, MD. Building Environment Div.
Simulation of an Evaporator with Nonuniform One-Dimensional Air Distribution.

Final rept. P. A. Domanski, 1991, 10p

Sponsored by Department of Energy, Washington, DC. Pub. in ASHRAE (American Society of Heating, Refrigerating and Air-Conditioning Engineers) Transactions, v97 pt1 10p 1991.

Keywords: \*Evaporators, \*Computerized simulation, \*Heat exchangers, \*Air conditioning, Heat transfer, Air flow, Mathematical models, Tubes, Mass transfer, Refrigerants, Dehumidification, Reprints.

The paper presents a simulation model of a plate-fin, air-to-refrigerant heat exchanger used as an evaporator in residential air conditioning. The model can account for nonuniform air distribution between coil tubes and simulates refrigerant distribution for coil circuits and individual tubes. The model is based on a tube-by-tube approach. Performance of each tube is analyzed separately by considering the cross-flow heat transfer with the external airstream and the appropriate heat and mass transfer relationships. Each tube is associated with individual refrigerant parameters and mass flow rate, and air mass flow rate, inlet

100,066

## Architectural Design & Environmental Engineering

temperature, and humidity. A comparison of the model's predictions and laboratory test data is provided. Simulation results indicate that air maldistribution may induce maldistribution of a refrigerant, which contributes to the performance degradation of the evapo-

100.067

PB91-175307 Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Building Physics Div.

Airtightness of Office-Building Envelopes. Final rept.

Sponsored by Department of Energy, Washington, DC.
Pub. in Proceedings of ASHRAE/DOE/BTECC Conference on Thermal Performance of the Exterior Envelopes of Buildings III, Clearwater Beach, FL., December 1985, p125-143.

Keywords: \*Ventilation, \*Office buildings, \*Leakage, \*Infiltration, \*Envelopes, Indoor air quality, Computerized simulation, Air flow, Pressure, Mathematical models, Energy consumption, Reprints.

Although airtightness, infiltration, and ventilation are important considerations in large office buildings, these issues have been studied less in office buildings than in residential buildings. Several features of office buildings make their air exchange characteristics dif-ferent from homes. These features include curtain wall design and construction, mechanical ventilation systems, specific occupancy patterns, large volumes and building heights, and low surface to volume ratios. The recent development of measuring procedures and computer simulation programs for large buildings has enabled the study of air leakage in large buildings and the effects of air exchange on energy use and indoor air quality. The paper discusses the airtightness and-building envelopes in modern office buildings and the relationship between envelope airtightness and air exchange rates. Results of whole building pressurization measurements and tracer gas measurements of air exchange rates in several office buildings are discussed, along with the relationship between these measurement results. A multizone computer simulation pro-gram developed at the National Bureau of Standards is applied to two office buildings to examine the relationship further. The results of the simulations reveal the importance of envelope airtightness, floor-to-floor cou-pling, and mechanical ventilation to the air change rates in these two buildings.

100,068

Final rept.

PB91-175471 Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Building Physics Div.

Measurement of Thermal Characteristics of Office Buildings.

L. K. Norford, A. Rabl, R. H. Socolow, and A. K. Persily. 1985, 17p

Sponsored by Department of Energy, Washington, DC. Pub. in Proceedings of ASHRAE/DOE/BTECC Conference on Thermal Performance of the Exterior Envelopes of Buildings III, Clearwater Beach, FL., December 1985, p272-288.

Keywords: \*Office buildings, \*Thermal measurements, \*Heat loss, Energy consumption, Heat transfer, Specific heat, Thermal analysis, Solar radiation, Heat transmission, Ventilation, Heating load, Reprints.

Thermal characteristics of two adjacent office buildings have been obtained from measurements of temperature, energy consumption and air exchange. The characteristics include the total heat-loss coefficient, a solar aperture, and building heat capacity. The heat-loss coefficient has been determined by steady state and transient analyses; transient analysis is required for the remaining characteristics. The effect of measured infiltration and ventilation rates on the total heatloss coefficient has been identified. Two methods have been used for the transient analysis: the egguivalent thermal paramter method of Sonderegger and the Fourier method of Subbarao.

#### 100.069

PR91-187286 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Building Environment Div

**BACnet Communication Protocol for Building Au**tomation Systems. Final rept.

S. T. Bushby, and H. M. Newman. 1991, 6p Pub. in ASHRAE (American Society of Heating, Refrig-eration and Air-Conditioning Engineers) Jnl., p14-15 and 18-21 Apr 91.

Keywords: \*Energy management systems, \*Protocol(Computers), \*HVAC systems, Communication networks, Data transmission, Standards, Automatic control, Buildings, Ventilation, Controllers, Reprints, \*Building Automation and Control network, \*BACnet.

The building community in the United States and in several other countries has been carefully watching the efforts by ASHRAE to develop a communication protocol for building energy management and control systems. The name of the standard protocol is 'BACnet' which stands for Building Automation and Control network. The article presents an overview of BACnet as it looks today and describes the tasks remaining to be completed. Control devices are modeled as a network-visible collection of objects. The information represented by these objects are accessed and manipulated through the use of a set of application layer services. The standard object-types that are defined and the application services included in the standard are described. Several possibilities for physical media and networking technology are being considered for inclusion in the standard. It is expected that BACnet will be released for public review by the end of January, 1991.

PB91-187732 PC A06/MF A01 National Inst. of Standards and Technology (BFRL), Gaithersburg, MD.
Draft Abstract Test Suite for Determining Con-

formance to the BACnet Protocol.

S. T. Bushby. Apr 91, 119p NISTIR-4563

Keywords: \*Protocol(Computers), \*Energy management systems, \*Buildings, Communication networks, Data transmission, Tests, Standards, Specifications, Control systems design, \*BACNET protocol.

The BACnet communication protocol for building auto-mation and control systems is in an advanced state of development and is expected to be released for public review in early 1991. When the review process is com-pleted it will become an ASHRAE standard. One of the important outstanding issues to be resolved is conformance to the standard and how to test devices to determine if they meet the conformance requirements. The report is a draft Abstract Test Suite based on working draft three of the proposed standard. The Abstract Test Suite is a first step in developing the tests which will be used to certify conformance to BACnet. Its purpose is to provide a starting point from which a conformance certification program can be built and to focus discussions on the outstanding conformance issues that need to be resolved before the standard can be considered complete. The role of an abstract test suite in the conformance testing process is described, a proposed BACnet test system architecture is presented and individual test cases are defined. Test cases to determine support for object types and application services defined in working draft three are included. A standard object configuration is also proposed to simplify the testing process.

100,071 PB91-187757 PC A04/MF A01 National Inst. of Standards and Technology (BFRL), Gaithersburg, MD.
Intelligent Building Technology in Japan.
A. Rubin. Apr 91, 69p NISTIR-4546

Sponsored by Department of Commerce, Washington, DC. Technology Administration, and Electric Power Research Inst., Palo Alto, CA.

Keywords: \*Buildings, \*Energy management systems, \*Japan, \*Technology assessment, Construction, Thermal energy storage systems, Environmental engineering, Ventilation, Air conditioning, Communication networks, \*Intelligent buildings, Office automation.

In May 1990, the author of the report visited Japan at the request of the Department of Commerce, to assess the Japanese experiences with 'intelligent building' design, construction and use. The state-ofthe-art was determined by visiting advanced buildings, building complexes, and interviewing architects, engineers, and researchers and academics. Discussions also were conducted with organizations engaged in promoting the use and design of intelligent buildings. In general, the Japanese experiences have paralleled those in the United States. In both countries, advanced building technologies have been employed to advance organizational effectiveness and personal productivity. A major problem shared by the two countries has been the lack of standardization of hardware and software (protocols), resulting in major difficulties in integrating equipment from different manufacturers, and in some instances, diverse products from the same manufacturer. Intelligent building design in Japan differs from that in the United States in several ways. They incorporate new systems and products into their buildings as soon as they become available. They stress the need for a high quality environment - amenity - more than we do. The commitment for developing improved intelligent buildings includes active governmental involvement by two major ministries and other institutions such as banks.

100,072 PB91-194936 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Building Environment Div. Rule-Based Diagnostic Method for HVAC Fault Detection. Final rept.

S. T. Liu, and G. E. Kelly. 1989, 6p Pub. in Proceedings of Building Simulation '89, Vancouver, British Columbia, Canada, June 23-24, 1989, p319-324

Keywords: \*HVAC systems, \*Energy management systems, \*Diagnostic techniques, Ventilation, Heating systems, Cooling systems, Defects, Control systems design, Signal detection, Reprints, \*Air handling units.

The paper describes the development of a prototype computerized diagnostic method for the detection of faulty equipment in an HVAC air handling unit (AHU) using sensor data from the building energy management system (BEMS) as input. The method uses a computer model of the AHU to compute a set of optimum performance parameters for the AHU under normal operating conditions and compares the parameters with actual values calculated from the measured sensor data. Deviations between the two sets of parameters are an indication of either an out-of-tune system or malfunction of certain equipment. The program will point out to the building operator the source of the fault and the possible cause in a timely fashion. The modeling part of the program is computation intensive and is written in the FORTRAN language. The diagnostic part is rule-based and is written in the symbolic language Prolog for its inference capability. Example case runs are presented to illustrate the proposed method.

100,073 PB91-195388 Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Building Environment Div.

Prediction and Fault Detection of Building Energy Consumption Using Multi-Input, Single-Output Dy-namical Model. Final rept.

J. Pakanen. 1988, 11p Sponsored by Technical Research Center of Finland, Helsinki, and Ministry of Trade and Industry, Helsinki

(Finland).
Pub. in Proceedings of International Symposium on Energy Options for the Year 2000 Contemporary Concepts in Technology and Policy, Newark, DE., September 14-17, 1988, v3 p3.57-3.67.

Keywords: \*Energy consumption, \*Buildings, Environmental engineering, Residential buildings, Space HVAC systems, Computerized simulation, Electrical faults, Degree days, Reprints.

For many years degree-days methods have been used to estimate building energy consumption. However, because degree-day method is based only on the outdoor temperature, there may be large differences between the actual and the calculated results. A new method is proposed, based upon on-line measurements of weather and other characteristic data. The method is capable of being used with building automa-tion systems for both failure detection and energy management applications. The method uses a multi-input, single-output (MISO) dynamical model to predict the power fluctuation of the building. The model parameters are identified recursively using measurements of the actual power, outdoor temperature, solar radiation, wind velocity and indoor tempeatures. Other

## **Architectural Design & Environmental Engineering**

measurements may also be used as input data. The stochastic variations in power caused by occupants, equipment, lights, etc, can be included in the model. Measurements are taken once an hour and are used to update the model parameters by a recursive extended least square algorithm (RELS). The identified model can be used to predict the energy consumption or to detect the failure of HVAC equipment and systems. Verification of the method has been accomplished using real weather data and the TARP-computer program for the simulation of buildings.

100,074 PB91-195438 PB91-195438 Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Building Equipment Div.

Diagnostic Techniques for Evaluating Office Building Envelopes. Final rept.

A. K. Persily, R. A. Grot, J. B. Fang, and Y. M.

Chang, 1988, 20p Sponsored by Public Buildings Service, Washington,

Pub. in Proceedings of ASHRAE (American Society of Heating, Refrigerating and Air-Conditioning Engineers) Winter Meeting, Dallas, TX., January 30, 1988, v94 pt1

Keywords: \*Office buildings, \*Diagnostic techniques, \*Thermal analysis, \*Energy conservation, Thermal insulation, Leakage, Heat flux, Transducers, Heat transmission, Thermal resistance, Reprints.

A variety of diagnostic procedures exists for evaluating the thermal performance of office building envelopes. These measurement techniques enable the quantifica-tion of various aspects of envelope thermal perform-ance including airtightness, thermal resistance, and insulation system performance. The paper describes several of these diagnostic measurement techniques in terms of instrumentation, test procedures, and data analysis. Representative measurement results are also presented for each technique. The techniques that are described include tracer gas measurements of the second air exchange rates, pressurization testing of whole building and component airtightness, thermal resistance measurements with calorimeter boxes and heat flux transducers, and infrared thermographic inspec-

100,075
PB91-206698
PC A03/MF A01
National Inst. of Standards and Technology (BFRL), Gaithersburg, MD. Indoor Ventilation Requirements for Manufactured

Housing. D. M. Burch. May 91, 29p NISTIR-4574

Sponsored by Department of Housing and Urban Development, Washington, DC.

Keywords: \*Ventilation, \*Indoor air pollution, Windows, Condensing, Environmental engineering, Formaldehyde, Air flow, Comfort, HVAC systems, Air quality, Houses, \*Manufactured housing.

In the study, a mathematical analysis is carried out to investigate the mechanical ventilation rates required in manufactured housing. The analysis reveals that the ventilation provided by natural infiltration is inadequate to comply with the ventilation requirements of ASHRAE Ventilation Standard 62-1889 and to prevent double-pane window condensation. The study recommends that both single-wide and double-wide mobile homes be equipped with mechanical ventilation equipment having a minimum installed capacity of 0.026 cu m/s (55 cu/min). It was found that considerably larger ventilation rates are needed to prevent condensation on single-pane windows. Therefore, it is recommended that double-pane windows be required in all heating climates.

100,076 PB91-206755 PC A06/MF A01 National Inst. of Standards and Technology (BFRL),

National Inst. of Standards and Technology (BFHL), Gaithersburg, MD.

Abstracts of Daylighting Research.

A. I. Rubin, R. Saraiji, R. McCluney, M. Huggins, and C. Emrich. May 91, 120p NISTIR-4578
Prepared in cooperation with Florida Solar Energy Center, Cape Canaveral. Sponsored by Electric Power Research Inst., Palo Alto, CA., and Lighting Research Inst., Palo Alto, CA., and Lighting Research

Inst., New York.

Keywords: \*Daylighting, \*Bibliographies, management, Computerized simulation, Mathematical models, Energy conservation, Glare, Abstracts.

The report is an annotated bibliography of Daylight research and practices. It is a compilation of two draft bibliographies, one compiled by the Florida Solar Energy Center, and the other by the National Institute of Standards and Technology. Both were the result of research projects conducted for the Electrical Power Research Institute. The topics covered are as follows: general treatments of daylight, energy saving design, research and design tools, control systems, computer, scale, and mathematical models, skylight research and applications, atria, fenestration systems and materials, shading devices, delivery systems--daylight and sunlight, and finally, the responses of people to light.

100,077 PB91-216655 PC A03/MF A01 National Inst. of Standards and Technology (BFRL), Variable Air Volume System Design Guide.
J. Y. Kao. Jun 91, 49p NISTIR-4605
Sponsored by Public Buildings Service, Washington,

Keywords: \*Office buildings, \*Ventilation, \*Air flow, \*Design criteria, Air conditioning, Environmental engineering, HVAC systems, Air circulation, Space heating, Control equipment.

Variable air volume (VAV) systems have been used ex-tensively in office buildings during recent years. How-ever, there are persistent complaints by building occupants about the air quality and environmental condi-tions of these buildings. The guide has been devel-oped to give guidelines on VAV system design to alle-viate possible design-caused problems. The guide pro-vides general discussion of VAV systems, air handling system design, system control, and commissioning. The guide has been developed for the General Services Administration to be used by GSA personnel and GSA's contract designers. It includes design check lists as a means of identifying major aspects in VAV system design where new construction and alteration of air systems are involved.

PB91-231563 PC A04/MF A01 National Inst. of Standards and Technology (BFRL), Gaithersburg, MD.

Daylight Research Requirements. Workshop Proceedings. Held in Baltimore, Maryland on August 1-2, 1990.

A. Rubin. Jul 91, 65p NISTIR-4639

Sponsored by Electric Power Research Inst., Palo Alto, CA., and Lighting Research Inst., New York, NY.

Keywords: \*Buildings, \*Daylighting, \*Meetings, Research and development, Computer aided design, Architecture, Windows, Energy efficiency, Technology transfer, Electric lighting, Design criteria, Commercial

The Daylighting Workshop was conducted on August 1-2, 1990 in Baltimore, Maryland. The overall purpose of the meeting was to develop a new research plan for daylighting, including interactions with other systems, such as electrical lighting and HVAC. The major objectives identified were to: determine the needs for new information (i.e. research); and suggest means of encouraging the application of daylighting, based on what is already known.

PB91-237800 Not available NTIS National Inst. of Standards and Technology (EEEL), Gaithersburg, MD. Electronics and Electrical Engineer-

ing Lab. Office.

Effect of Veiling Relections on Vision of Colored Objects.

Final rept

J. A. Worthey. 1989, 6p Pub. in Jnl. of the Illuminating Engineering Society 18, n2 p10-15 1989.

Keywords: \*Illunimating, \*Buildings, Research and development, Reflection, Light sources, Color, Reprints.

Familiar light sources vary greatly in the solid angle they subtend. A recent paper examined the effect of light source size, and quantified the obvious facts that a small source makes veiling reflections brighter, but a large source makes them harder to avoid. One conclusion was that veiling reflections are never negligible. The present paper pursues this idea by quantifying the effect of surface reflections on vision of colored objects. It is found that speerical lighting reduces the range of colors seen in glossy objects by 37%. 100,080

PR91-237818 Not available NTIS National Inst. of Standards and Technology (EEEL), Gaithersburg, MD. Electronics and Electrical Engineering Lab. Office.

Light Source Area, Shading, and Glare.

Final rept.

Pub. in Jnl. of the Illuminating Engineering Society 20, n2 p29-36 1991.

Keywords: \*Light sources, \*Illuminating, Glare, Reflection, Luminance, Research management, Reprints.

Familiar light sources vary in the solid angle they sub-tend by a factor of 100,000 or more. The effects of source area on object shading and on direct illumination of the eye are examined through simplified examples. Previous papers have looked at highlights and veiling reflections in a similar way.

100.081

PB91-237826 Not available NTIS National Inst. of Standards and Technology (EEEL), Gaithersburg, MD. Electronics and Electrical Engineering Lab. Office.

Role of Theory in Lighting Research and Design. Final rept.

J. A. Worthey. 1991, 3p Pub. in Lighting Design and Application 21, n7 p15-17 Jul 91.

Keywords: \*Illuminating, \*Research management, Spectra, Light sources, Design, Theories, Luminance, Reprints.

Although science in general acknowledges the role of theory, the need for theoretical methods is not so well established in the case of lighting research and design. Among the reasons that theory is important to lighting work are these: (1) Theory is what engineers do. (2) It is hard to vary light-source size. (3) It is also hard to vary Spectral Power Distribution. (4) Optics is not controversial. (5) Theory guides experiment. (6) More speculative theories also have a place.

100 082

PB91-240747 PC A04/MF A01 National Inst. of Standards and Technology (BFRL), Gaithersburg, MD.

Preliminary Results of the Environmental Evaluation of the Federal Records Center in Overland

A. K. Persily, W. S. Dols, S. J. Nabinger, and S. Kirchner. Jul 91, 52p NISTIR-4634 Sponsored by Public Buildings Service, Washington, DC.

Keywords: \*Federal buildings, \*Environmental engineering, Indoor air pollution, Air infiltration, Air quality, Carbon dioxide, Carbon monoxide, Formaldehyde, Radon, Ventilation, Missouri.

The National Institute of Standards and Technology (NIST) is studying the thermal and environmental performance of new federal office buildings for the Public Buildings Service of the General Services Administrabuildings service of the derief at Services Administra-tion (GSA). The project involves long-term perform-ance monitoring both before occupancy and during early occupancy in three new office buildings. The per-formance evaluation includes an assessment of the thermal integrity of the building envelope, long-term monitoring of ventilation system performance, and the measurement of indoor levels of selected pollutants. The report describes the effort being conducted in the second of the three buildings, the Federal Records Center in Overland Missouri, and presents preliminary measurement results from the building. The infrared thermographic inspection of the Overland Building did not reveal any significant thermal defects in the building envelope, though the existence of air leakage and thermal bridging was noted. The whole building pressurization test showed that the building is quite leaky compared to other modern office buildings. The meascompared to other modern office buildings. The measured radon concentrations were 2 pCi/L or less on the B2 level, and less than or equal to 0.5 pCi/L on the other levels. Formaldehyde concentrations ranged from 0.03 to 0.07 ppm, below the 0.1 ppm guideline but above some levels of concern. The measured levels of volatile organic compounds were similar to those observed in other peut office buildings must be considered. served in other new office buildings, and the impact of building furnishings and construction activities on the VOC levels were noted. The carbon dioxide levels in

100,082

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the building have generally been low, as would be expected in a building with low levels of occupancy.

#### **Building Equipment, Furnishings, &** Maintenance

100,083 PB91-161984 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Building Environment Div.

Visibility of Exit Signs and Directional Indicators. Final rept.

B. L. Collins. 1991, 17p Sponsored by National Electrical Mfrs. Association, Washington, DC.

Pub. in Jnl. of the Illuminating Engineering Society, p117-133 1991.

Keywords: \*Sign visibility, \*Exits, \*Direction signs, Visual perception, Color, Signal visibility, Visual threshold, Signs, Contract, Sign effectiveness, Sign colors,

A three-phase experiment assessed the visibility of exit signs and directional indicators. Sign effectiveness was determined in terms of distance to detection, cor-rect identification, and rated effectiveness, as well as speed through a corridor in one phase. The results indicated that a 2.25-in. chevron in grey on white with a contrast of about 0.5 (to meet minimum specifications) was identified correctly at the greatest mean distance and received the highest mean ratings of effectiveness, compared to other indicators. The combination of a 2.25-in. chevron with a 6-in. EXIT sign was identified correctly at a mean distance of about 100 ft. Use of color, either red or green increased the identification distance by about 15 to 20 ft. Reducing width to height ratio reduced identification distance by about 35-40 ft. for chevrons of comparable height, although chevrons of 2.6 to 3.75-in. in height, with a width to height ration of 0.29 to 0.43, were identified correctly at about 100 ft. These data suggest that chevron width can be reduced if height is increased beyond 2.6-in. to maintain adequate visibility at 100 ft. The data indicate the importance of chevron size and configuration as well as sign color and contrast in determining visibility.

PB91-187260 Not available NTIS National Inst. of Standards and Technology (BFRL), Gaithersburg, MD. Improving the Fire Performance of Building Con-

Final rept.

R. W. Bukowski. 1991, 5p

Pub. in Construction Specifier 44, n2 p42-46 Feb 91.

Keywords: \*Building codes, \*Fire resistant materials, \*Flammability, Furniture, Fire tests, Standards, Measurement, Risk assessment, Hazards, Upholstery, Re-

This is a short article for The Construction Specifier magazine which reviews current activities relative to the regulation of building contents, e.g., upholstered furniture, mattresses, drapes, etc. It reviews the current status of California Technical Bulletin 133, UL, and NFPA standardization activities. The role of computer fire models and measurement methods in providing the data for them in the context of such regulation is discussed.

100,085 PB91-189274 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Building Environment Div.

Measured Performance of Residential Water Heaters Using Existing and Proposed Department of Energy Test Procedures. Final rept.

A. H. Fanney, 1990, 8p Sponsored by Department of Energy, Washington, DC. Pub. in ASHRAE (American Society of Heating, Refrigerating and Air-Conditioning Engineers) Transactions, v96, pt1 p288-295 Jan 90.

Keywords: \*Water heaters, Residential buildings, Laboratories, Experimental design, Computerized simulation, US DOE, Standards, Reprints.

computer-based laboratory for testing residential water heaters has been fabricated at the National Insti-

tute of Standards and Technology (NIST). The paper describes the automated laboratory, summarizes existing and proposed Department of Energy test procedures for residential water heaters, and presents ex-perimental results for six electric, five gas-fired, and two oil-fired storage-type water heaters obtained from local distributors.

100,086
PB91-206664
PC A08/MF A01
Dayton Univ., OH. Research Inst.
Technical Reference and User's Guide for FAST/ FFM Version 3.

Technical rept. (Final) M. A. Dietenberger, May 91, 153p NIST/GCR-91/

Grant NANB-SD-0557

Sponsored by National Inst. of Standards and Technology (BFRL), Gaithersburg, MD.

Keywords: \*Fires, \*Furniture, \*Burning rate, \*Combustion products, \*User manuals(Computer programs), Buildings, Smoke, Mathematical models, Compartments, Combustion, Heat flux, FAST/FFM computer program.

The FAST/FFM computer model provides dynamic, quasi-three-dimensional predictions of furniture fire growth and burnout in a room as well as of the spread of both nontoxic and toxic gases, smoke, and fire to other rooms. The reference guide provides a detailed description of the furniture fire model (FFM) equations, the program structure of FFM and its insertion into FAST, the FFM data input requirements, and the output produced by version 3 of the model.

100,087 PB92-108984 National Inst. of Standards and Technology (BFRL), Gaithersburg, MD.

Cone Calorimeter Rate of Heat Release Measurements for Upholstered Composites of Polyure-thane Foams.

K. M. Villa, and V. Babrauskas. Aug 91, 40p NISTIR-4652

Keywords: \*Fire tests, \*Upholstery, \*Polyurethanes, Combustion products, Fire hazards, Furniture, Chairs, Thermal measurements, Calorimeters, Cone calorimeters.

Certain regulatory authorities have recently banned or restricted the use of furniture upholstered with a combination of polyvinyl chloride (PVC) covering and a melamine-treated polyurethane foam padding. Thus, it was endeavored to determine if quantitative measurements would reveal any special hazards associated with this particular combination. The work represents the testing of nine different upholstered composites, made of fabric coverings and polyurethane foam, tested at three different irradiance levels in the National Institute of Standards and Technology Cone Calo-rimeter. Additional combinations using a polyester bat-ting interbarrier were also used. The composite bench-scale specimens were tested at 25 kW/sq.m, 35 kW/ sq.m and 50 kW/sq.m irradiance levels. For most variables describing fire hazard, the performance of the combination of melamine-treated polyurethane foam and PVC fabric covering was not found to behave in an unusual manner. Only by considering the time period of 15 seconds after ignition was this combination numerically worse than all other combinations tested

100.088 PB92-109156 PC A09/MF A02 National Inst. of Standards and Technology (BFRL), Gaithersburg, MD. International Fire Detection Bibliography, 1975-

**1990.** R. W. Bukowski, and N. H. Jason. Sep 91, 185p NISTIR-4661

See also COM-74-50638. Sponsored by National Fire Protection Research Foundation, Quincy, MA.

Keywords: \*Bibliographies, \*Fire detection systems, \*Smoke detectors, \*Fire alarm systems, Fire protection, Abstracts, Fire detectors, Sprinkler systems, Gas detectors, Fire safety, Safety devices.

The bibliography was collected from numerous international sources and represents as complete a compilation of publications from the 15 years covered as could be collected. Nearly 1000 references are included, separated into one of 20 topics such as aerosols and smoke, industrial occupancies, ships, smart detectors and systems, and system reliability studies. Each

such section begins with a brief summary and cites the more important papers within. The bibliography ends with a commentary on what the overall literature shows, what research is needed to achieve more reliable detection system operation and reduced unwanted alarms. An author index and a key word index are provided.

#### **Building Standards & Codes**

100,089 PB91-190066 Not available NTIS National Inst. of Standards and Technology, Gaithersburg, MD. Lab. Accreditation Program. Plumbing Test Lab Accreditation.

Final rept.

J. A. Swaffield, and L. S. Galowin. 1991, 5p Pub. in Heating/Piping/Air Conditioning 63, n3 p73-77

Keywords: \*Plumbing, \*Building codes, \*Test facilities, \*Accreditation, Piping systems, Standards, Water conservation, Test methods, Drainage, Performance, Pipes(Tubes), Reprints.

The ability to evaluate plumbing laboratory competency for conducting tests established in standards is assured through the accreditation of testing laboratories. The National Voluntary Laboratory Accreditation Program (NVLAP) of the National Institute of Standards and Technology (NIST) has announced Plumbing Accreditation as an addition to the Commercial Products Testing Program. NVLAP provides recognition for lab-oratory competence and support for objectivity in test-ing and thereby assists industry in interstate com-merce. Procurement officials, designers, specifiers and water conservation managers and planners can specify that test data show conformance to specificaspecify that test data show combinated to specifica-tions in standards in reports for performance of plumb-ing devices are from NVLAP accredited laboratories. The accreditation process for determining the qualifi-cations for testing laboratories are described. Applications of research for drainage systems and plumbing products are discussed for input to plumbing codes and standards for pipe sizing are shown from experiments and computer model determinations related to pipe pitch and diameter for waste transport.

100 090 PB91-194811 Not available NTIS National Inst. of Standards and Technology (BFRL),

Gaithersburg, MD.
Meeting the Challenges of a Global Market - Construction Standards, Testing and Certification. Final rept.

J. G. Gross. 1991, 4p Pub. in Construction Business Review, p31-34 Mar/

Keywords: \*Standards, \*Construction materials, \*Europe, \*International trade, Test methods, Product development, Certification, Competition, Regulations, Reprints, European Economic Community.

The article provides information on the rapidly changing global market for construction products and services. Particularly, the unification of the European Community and activities in the development of the EC 92 internal market are discussed. Standards development processes in the United States and internationally are reviewed. The importance of standards as the basis for requisition and commerce makes these activities. for regulation and commerce makes these activities extremely important for the U.S. design profession and building product producers. Related testing, certification and product approval requirements are reviewed. Recommendations for the U.S. construction community are provided.

PB91-216614 PC A03/MF A01 National Inst. of Standards and Technology (BFRL), Gaithersburg, MD.

Direct Digital Control Based Building Automation

System Design Criteria.
J. Y. Kao. Jun 91, 37p NISTIR-4604
Sponsored by Public Buildings Service, Washington,

Keywords: \*Digital command systems, \*Automatic control, \*Federal buildings, Public buildings, Energy

#### **Building Standards & Codes**

management systems, Quality control, HVAC systems, Fire protection, Security, Controllers, Warning systems, Design criteria, Guidelines, Specifications, \*Direct digital control, \*Building automation control.

The document serves to provide design guidance for Direct Digital Control (DDC) based Building Automation Systems (BAS). It also provides instructions to design engineers for the BAS design. Explanations of general design philosophy, current unresolved prob-lems confronting the application of DDC in BAS, and considerations for choosing alternative control strategies in specifying application programs are given. The guide is intended for use by GSA and contract designers as a means of identifying major aspects in DDC based BAS design where new construction or major renovations of control systems are included.

100,092 PB91-216697 PC A04/MF A01 National Inst. of Standards and Technology (BFRL), Gaithersburg, MD.

Guide Specification for Direct Digital Control

Based Building Automation System.

J. Y. Kao. Jun 91, 72p NISTIR-4606
Sponsored by Public Buildings Service, Washington,

Keywords: \*Specifications, \*Digital command systems, \*Automatic control, \*Federal buildings, Energy management systems, Warning systems, Fire protection, Controllers, HVAC systems, Security, Quality assurance, Design criteria, Public buildings, \*Building automation systems, \*Direct digital control.

The publication is intended for building system designers' use in specifying direct digital control (DDC) based building automation systems (BAS) for construction of Federal buildings. The guide specification conforms with the format of guide specifications used by the General Services Administration (GSA) and its professional services contractors.

#### Construction Materials, Components, & Equipment

100,093 PB91-132134 PC A03/MF A01 National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Center for Fire Research. Concept of the Calculus of Fire Safety. R. L. Smith. Nov 90, 23p NISTIR-4459

Keywords: \*Fire safety, \*Buildings, Artificial intelligence, Statistical analysis, Probability theory, Burns(Injuries), Death, Fire hazards, Computer systems programs, \*Risk assessment, Expert systems.

Many people (builders, owners, designers, occupants, etc.) have an interest in appraising the fire safety of existing or proposed buildings. Computers are playing an ever increasing role in fire safety analysis and in the technology transfer of fire science. In the report the concept of the Calculus of Fire Safety is developed as a declarative programming language. This calculus will enable users to specify what fire safety question is to be answered without specifying how the answer is to be obtained. Advances in Artificial Intelligence programming techniques will enable the implementation of the Calculus of Fire Safety on widely available workstations. This will provide a very powerful tool to anyone interested in determining the fire safety of buildings.

PB91-143297 PC A04/MF A01 Pennsylvania State Univ., University Park. Dept. of Mechanical Engineering.
Heat Flux, Mass Loss Rate and Upward Flame

Spread for Burning Vertical Walls (1990).

Annual rept. A. K. Kulkarni, C. I. Kim, and C. H. Kuo. Nov 90, 65p

NIST/GCR-90/584
Grant NANB8D0849
Sponsored by National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Center for Fire Re-

Keywords: \*Heat flux, \*Walls, \*Fire tests, \*Flames, Burning rate, Mathematical models, Construction materials, Test facilities, Conduction, Heat transfer, Heat Progress made during the first year of NIST Grant No. 60NANB8D0849 for the period ending August 14, 1989 is reported here. The overall objective of the grant is to understand the basic mechanisms of upward flame spread and to develop a methodology to predict the flame spread on practical wall materials, approximately verified by experiments. In the report, progress made on the following tasks is described in individual sections, upward flame spread experiments, mathematical model, local mass loss rate apparatus, heat conduction in the interior of burning walls, and Gardon heat flux gage calibration.

PB91-144394 PC A03/MF A01 National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Center for Fire Research. Using the Harvard/NIST Mark VI Fire Simulation. J. A. Rockett. Nov 90, 45p NISTIR-4464

Keywords: \*Fires, \*Computerized simulation, \*Buildings, Burning rate, Combustion, Plumes, Entrainment, Walls, Algorithms, Flames, \*Harvard/NIST VI computer program

Installation and use of the Harvard/NIST multi-room fire simulation (computer code on the IBM PC (and compatibles) is described. Two separate auxiliary programs, MASBANK and PREPLOT are also described and their use illustrated. Use of the input menus is described and illustrated. Comments are made on the effect of the choice of alternative sub-models on predicted results. Some suggestions for use on other computers are made. The H06.3 disks for use with the report include: Disk No. 1: All files (in packed form) report include: Disk No. 1: All lites (in packed form) needed to run Ho6.3 and the two auxiliary programs: MASBANK and PREPLOT. A group of (packed) files including a short data base file and a sample output of Ho6.3. Disk No. 2: Section 1 including 17 out of 25 source code files for Ho6.3. Disk No. 3: Section 2 including 17 out of 25 source code files for Ho6.3. Disk No. 3: Section 2 including 17 out of 25 including 17 out of 25 including 18 output of 25 include 18 output of 25 including 18 output of 25 including 18 output of 25 including 18 output of 25 include 18 output of 25 include 25 include 18 output of 25 include 25 cluding the final 8 source code files of H06.3 and source code for MASBANK, PREPLOT and the auxiliary source code file DTIME.

100.096 PB91-144436 PC A06/MF A01 National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Center for Fire Research. Programmer's Reference Manual for CFAST, the Unified Model of Fire Growth and Smoke Transport. Technical note (Final).

W. W. Jones, and G. P. Forney. Nov 90, 107p NIST/TN-1283

Also available from Supt. of Docs. as SN003-003-03041-4.

Keywords: \*Smoke, \*Fires, \*Buildings, Mathematical models, Combustion, Transport properties, Combustion products, Computer applications, Plumes, Pyrolysis, Programming manuals, Protocols, Data file, Software engineering, Computer programs, CFAST computer program.

The document describes the unified model of fire growth and smoke spread, CFAST. The paper documents the internal structure of the model and details the method of modifying the model, together with examples. The intent is to provide a framework and methodology for maintenance of the model, together with a method of updating it. The reader is assumed to have a working knowledge of programming, software maintenance and modeling of physical phenomena.

100.097 PB91-146977 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Fire Measurement and Research

Heat Release Rate: The Single Most Important Variable in Fire Hazard. Final rept.

V. Babrauskas, and R. D. Peacock. 1990, 14p Pub. in Proceedings of Fall Meeting Fire Safety Developments and Testing: Toxicity, Heat Release, Product Development, Combustion Corrosivity, Fire Retardant Chemicals Association, Ponte Vedra Beach, FL., October 20-25, 1990, p67-80.

Keywords: \*Fire hazards, \*Heat of combustion, \*Fires, Ignition, Combustion, Fire tests, Burning rate, Thermodynamic properties, Heat transfer, Heat flux, Flammability, Reprints, \*Heat release rate.

Heat release rate measurements are sometimes seen by manufacturers and product users as just another

piece of data to gather. It is the purpose of the paper to explain why heat release rate is, in fact, the single most important variable in characterizing the 'flamma-bility' of products and their consequent fire hazard. Examples of typical fire histories are given which illustrate that even though fire deaths are primarily caused by toxic gases, the heat release rate is the best predictor of fire hazard. Conversely, the relative toxicity of the combustion gases plays a smaller role. The delays in ignition time, as measured by various Bunsen burner type tests, also have only a minor effect on the development of fire hazard.

100.098 PB91-147215 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Fire Science and Engineering Div.

Review of Four Compartment Fires with Four Compartment Fire Models.

Final rept. S. Deal. 1990, 20p

Pub. in Proceedings of Fire Retardant Chemicals Association/Fire Safety Developments and Testing Fall Conference, Ponte Vedra Beach, October 21-24, 1990, p1-20.

Keywords: \*Fires, \*Compartments, \*Models, Air flow, Fire tests, Ventilation, Buildings, Interfaces, Fuels, Gas flow, Combustion, Reprints.

A comparison of four compartment zone fire models (FIRST, FAST, CCFM VENTS and FPETOOL) is presented with four experimental compartment fires. The four experiments represent a variation of vent and fuel effects upon the fire. The models were compared with regard to their simulated temperature, oxygen concentration, interface height and vent flow. Overall, the models compared well with the experimental data, but some discrepancies existed. These are discussed. The models are qualitatively ranked with regard to the amount of fire science knowledge the user should possess and the detail with which the simulation is pur-

100.099 PB91-147439 Not available NTIS National Bureau of Standards (NEL), Gaithersburg,

MD. Building Materials Div.

Design of High Strength Cement-Based Materials.

Part 2. Microstructure.

Final rept.

H. M. Jennings. 1988, 6p See also PB90-152653. Sponsored by Air Force Engineering and Services Center, Tyndall ÁFB, FL. Pub. in Materials Science and Technology 4, n4 p285-290 Apr 88.

Keywords: \*High strength concretes, \*Cements, \*Microstructure, Strength, Mechanical properties, Toughness, Fracture properties, Concrete durability, Fractures (Materials), Fracture strength, Design criteria, Reprints.

The report is Part II of a three part paper that examines relationships between microstructure and strength of cement-based materials. Microstructural fracture that may be related to strength are discussed.

PB91-147611 Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Building Environment Div. Temperature Measurement of Glass Subjected to Solar Radiation.

Final rept.
S. T. Liu. 1988, 10p
Pub. in ASHRAE (American Society of Heating, Refrigerating and Air-Conditioning Engineers) Transactions 94, pt2 p1350-1359 1988.

Keywords: \*Windows, \*Temperature measurement, \*Solar radiation, Radiative heat transfer, Temperature measuring instruments, Thermal radiation, Thermo-couples, Glass coatings, Window glazing, Reflectance, Reprints.

The measurement of the temperature of window glass exposed to direct solar radiation was studied experimentally under clear sky conditions. Thermocouples of different constructions were mounted on the surface of a 3.18 mm (1/8-inch) window glass panel and their outputs were monitored simultaneously under both direct solar radiation and shaded conditions. The thermocouples used for the experiment were a pair of thin foil type with butt-bonded bare metal junction, a pair of

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thin foil type encased in thin polymer/glass laminates, and a 40 gauge wire, beaded junction. For the foil types, one from each pair was coated with a highly reflective white paint. Shading was applied after stable output was established, and responses from the step change in irradiation level were recorded. It was found that there can be a 0.2 to 0.7C difference in the measured temperature for the glass surface between a bare metal junction and a junction coated with a high reflec-tivity (in the shortwave spectrum) paint. The difference in indicated temperature between an unpainted lami-nated junction and a painted junction can be as high as 1.0C. The radiative properties of the junction's surface, both in the solar and the infrared spectrum, are shown to have equal effect on the surface temperature meas-

100,101 PB91-147835 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Fire Measurement and Research

Forced Smolder Propagation and the Transition to Flaming in Cellulosic Insulation.

Final rept.

Final rept.
T. J. Ohlemiller. 1990, 12p
See also PB86-166657. Sponsored by Department of Energy, Washington, DC.
Pub. in Combustion and Flame 81, n3-4 p354-365 Sep

Keywords: \*Thermal insulation, \*Flame propagation, \*Flammability testing, Cellular materials, Construction materials, Combustion, Ignition, Air flow, Reaction kinetics, Fire resistant materials, Flash point, Reprints.

It is well known that a smoldering fuel responds to an It is well known that a smoldering fuel responds to an increased oxygen supply by becoming faster and hotter until, eventually, flames erupt. The sequence was examined quantitatively for thick horizontal layers of a permeable fuel, i.e., cellulosic insulation. Two configurations are possible, forward and reverse smolder, both were investigated experimentally. Reverse smolder was shown to respond only weakly to an increased air flow and it selvibility no transition. It domine at flow air flow and it exhibited no transition to flaming at flow velocities up to 5 m/s. Forward smolder responded strongly to increased air flow and yielded transition to flaming at about 2 m/s for unretarded material. The influence of combustion retardants was also examined, these included boric acid, a smolder retardant, and borax, a flaming retardant. Both prevented the transition to flaming in the absence of adjacent flammable material but were less effective in its presence. The overall response of these various fuel mixtures and configurations suggests that both kinetics (via leading edge heat transfer effects) and oxygen supply rate (not the latter alone) play substantial roles in dictating smolder response to an air flow.

100,102 PB91-147843 PB91-147843 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Fire Measurement and Research

Smoldering Combustion Propagation Through a Permeable Horizontal Fuel Layer. Final rept.

That Tept.

T. J. Ohlemiller. 1990, 13p
Sponsored by Department of Energy, Washington, DC.
Pub. in Combustion and Flame 81, n3-4 p341-353 Sep

Keywords: \*Flammability testing, \*Thermal insulation, \*Flame propagation, Flammability, Fire resistant materials, Combustion, Ignition, Reaction kinetics, Pyrolysis, Combustion products, Air flow, Reprints.

Although the propagation rate of smoldering through porous horizontal fuel layers has been measured for a variety of materials, there has been little work on the structure of the smolder reaction zone and the factors controlling it. These latter aspects are the focus here for the case of thick (18 cm) layers of wood-based fibers in the form of cellulosic insulation smoldering under natural convection air supply conditions. Two-dimensional profiles of temperature, oxygen mole fraction, and residual organic material have been measured both for unretarded insulation and for insulation having 25 wt% of the smolder retardant, boric acid, added on. It is inferred that the overall wave structure added off. It is illerted that the overall wave structure is dominated by oxygen diffusion from above. The heat release chemistry appears to involve both oxidative pyrolysis and char oxidation in a shifting balance depending on depth in the layer. Boric acid is unable to halt the smolder process in these thick fuel layers but it slows its spread by about a factor of 2 by a combination of oxidations. tion of endothermic and kinetic effects.

100.103 PB91-147975 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Building Equipment Div. Evaluation of Fumed-Silica Insulation for a Thermal Conductivity Standard Reference Material.

B. G. Rennex, T. A. Somers, T. K. Faison, and R. R. Zarr. 1990, 12p Sponsored by Department of Energy, Washington, DC.

Office of Buildings Energy R and D.
Pub. in Insulation Materials, Testing, and Applications,

ASTM STP 1030, p3-14 1990.

Keywords: \*Thermal insulation, \*Thermal conductivity, \*Silicon dioxide, Thermal resistance, Conductive heat transfer, Heat measurement, Test facilities, Temperature effects, Thermodynamic properties, Heat treatment, Heat transfer, Reprints, \*Standard reference

Standard Reference Materials (SRMs) used for thermal conductivity measurements are required by industry, academic, and government laboratories for calibrating heat-flux-meter apparatus or checking the ac-curacy of guarded-hot-plate apparatus. New thermal conductivity SRMs are sought to improve the accuracy and extend the operational range of these apparatus. An advisory panel recommended the development of a low thermal conductivity SRM having approximately the same thermal conductivity as blown fluorocarbon foams, suitable for a temperature range of -175 to 900 C. The National Bureau of Standards (NBS) examined four lots of fumed-silica insulation and recommended one candidate for further development as a low ther-mal conductivity SRM. The four lots of fumed-silica in-sulation were examined for their relative handleability, material uniformity, variability of thermal conductivity measurements, and effect of heat treatment on the measured thermal conductivity of the materials. Thermal conductivity measurements were conducted using the NBS 1-m Guarded Hot Plate for each lot of fumedsilica insulation at a mean specimen temperature of 24C. Analysis of the thermal conductivity data was performed using the NBS statistical analysis program, Dataplot.

100.104 PB91-148510 PC A04/MF A01 National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Center for Fire Research. Refinement of a Model for Fire Growth and Smoke Transport.

Technical note (Final).
W. W. Jones. Nov 90, 53p NIST/TN-1282
Also available from Supt. of Docs. as SN003-003-

Keywords: \*Fires, \*Smoke, \*Buildings, \*Mathematical models, Fire hazards, Ventilation, Combustion products, Computer applications, Transport properties, Pyrolysis, Mass flow, Computer programs, Data file, Toxicity, Deposition, Hydrogen chloride.

The document describes the changes which have occurred in FAST, FASTplot, FAST in and the distribution disks in the change from 18.3, the release for Hazard I, and the current release 18.5. Included are an errata section for the Technical Note 1262, a revision history that is distributed with the release disks, the addendum to the Technical Note for the new key words, and the description of the implementation of the physical rou-

PB91-149153 Not available NTIS Mational Bureau of Standards (NEL), Gaithersburg, MD. Building Materials Div.

Further Investigation of the Effect of Application Parameters on Adhesive-Bonded Seams of Single-Ply Roof Membranes.

Final rept.

W. J. Rossiter. 1988, 7p Sponsored by Corps of Engineers, Washington, DC. Pub. in Materials and Structures 21, p243-249 1988.

Keywords: \*Roofing, \*Adhesive bonding, \*Ethylene propylene diene polymers, \*Peel tests, Synthetic elastomers, Process variables, Temperature dependence, Time dependence, Pressure dependence, Surface finishing, Seame(Joints), Quality assurance, Reprints.

A laboratory study was conducted to determine if a Tpeel test was sensitive to differences in initial (7 days) bond strength for adhesive-bonded seams of EPDM

(ethylene propylene diene terpolymer) rubber membranes made under different application conditions. The main categories of application parameters investigated were: surface condition (cleanness, moisture) of the rubber; pressure applied; temperature during seam formation; open time. The T-peel test was found to be sensitive to changes in bond resulting from variation of some of the application parameters. Seams prepared using uncleaned sheets (without removing the talc or contaminants from their surfaces), or using long open times, had lower average peel strengths than those of the control specimens. Light pressure or high those of the control specimens. Light pressure or high temperature during bond formation produced seams with average peel strengths higher than those of the controls. Wet surfaces and low temperature had no significant effect on the average strength of the seams. The result that uncleaned surfaces had reduced T-peel strength was significant in that lack of proper surface preparation has been cited as a major tester. factor affecting seam performance in service. This result suggested that the T-peel test offers promise for use in developing a quality assurance methodology to assess whether field-prepared seams are made in accordance with acceptable practice.

100.106

PB91-157172 PC A03/MF A01 National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Center for Building Technology. Pulse-Echo Ultrasonic Evaluation of the Integrity of Seams of Single-Ply Roofing Membranes: Laboratory Evaluation of a Prototype Test Apparatus. H. Watanabe, and W. J. Rossiter. Dec 90, 47p NISTIR-4424

Prepared in cooperation with Takenaka Corp., Tokyo (Japan). Technical Research Lab. Sponsored by Civil Engineering Lab. (Navy), Port Hueneme, CA.

Keywords: \*Ultrasonic tests, \*Test facilities, \*Roofing, \*Seams(Joints), \*Adhesive bonding, Transducers, Acoustic measurement, Construction materials, Mem-branes, Adhesion, Voids, Prototypes, Pressure, Non-destructive tests, \*Single-ply roofing membranes.

The feasibility of using NDE (non-destructive evaluation) methods to detect voids in adhesive-bonded seams of single-ply membranes has been under investigation at the National Institute of Standards and Technology (NIST). The report covers the first phase of a two-part study to investigate the applicability of a pulse-echo ultrasonic method for this purpose. A prototype pulse-echo ultrasonic apparatus, called the field scanner and suitable for testing of single-ply seams in the field, was developed. A series of laboratory experiments was conducted using the field scanner to investigate: (1) optimal operating conditions, (2) sensitivity and practical limitations for detecting voids, and (3) variables affecting its response. The equipment was found to be effective in maintaining coupling between the transducer and seam specimens. Two 5-MHz transducers (focusing and non-focusing types) were selected as the most suitable for void detection in the seams. Voids incorporated in laboratory seam specimens were readily detected. The results of the Phase mens were readily detected. The results of the Phase 1 investigation provided guidelines on the optimum conditions for use of the field scanner. Although not without limitations, encouraging evidence was ob-tained indicating that the field scanner should be appli-cable to inspections of EPDM seams in service. Con-sequently, field investigations are being conducted, as planned, in Phase 2 of the study.

100,107

PB91-158543 Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Fire Safety Technology Div.

Compartment Fire-Generated Environment and

Smoke Filling.

Final rept.

Public Projection Engineering, Chapter 7, p2-116-2-138 1988.

Keywords: \*Smoke, \*Fires, \*Mathematical models, \*Buildings, \*Air flow, Combustion products, Ventilation, Fire safety, Hazards, Fire protection, Reprints.

The Chapter describes some of the key phenomena which occur in compartment fires, and it focuses on Smoke Filling which is one of the simplest quantitative global descriptions of these phenomena. A specific smoke filling model is presented, and solutions to its model equations are discussed along with example applications.

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100,108 PB91-158998 PB91-158998 Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Fire Safety Technology Div.

Algorithm for the Mass-Loss Rate of a Burning

Wall.

Final rept

H. E. Mitler. 1989, 10p

Pub. in Proceedings of the International Symposium on Fire Safety Science (2nd), Tokyo, Japan, June 1988, p179-188 1989.

Keywords: \*Algorithms, \*Burning rate, \*Fires, \*Walls, Pyrolysis, Thermophysical properties, Buildings, Fire safety, Mathematical models, Reprints.

A derivation is given for a simple algorithm which yields the quasi-steady burning rate of a verticle panel of non-charring, non-melting material in an enclosure with stratification of temperature and oxygen concen-tration. The algorithm requires the solution of a transcendental equation. Among the thermophysical data which are needed, are the mean flame temperature and the height-dependent absorption coefficient. It is found from experiment that the absorption coefficient is well described for PMMA by a two-parameter expression linear in 1/z. Comparison with a transient experiment yields good agreemtn for the mass-loss rate, over much of the range.

PB91-159038 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Fire Measurement and Research

Five Small Flaming Fire Tests in a Simulated Hospital Patient Room Protected by Automatic Fire Sprinklers.

K. A. Notarianni. 1990, 23p Pub. in Report of Test FR 3982, p1-23, 31 Oct 90.

Keywords: \*Fire tests, \*Hospitals, \*Sprinklers, \*Fire protection, Fire damage, Fire safety, Sprinkler systems, Fire fighting, Design criteria, Reprints.

A series of five tests were conducted to measure temperatures, radiation, and carbon dioxide, carbon monoxide, and oxygen concentrations resulting from small flaming wood crib fires within a simulated NIH hospital patient room protected with automatic fire sprinklers. Time to activation of quick and standard response sprinklers and ionization and photoelectric smoke de-tectors at several locations in the room simulating multiple options for protection of the space were measured. The test series addressed the location of sprinkler heads in the hospital patient room, demonstrated the effect of privacy curtains around the beds, the effect of a shielded fire, and the effect of sidewall sprinklers.

100,110 PB91-159731 PC A03/MF A01 National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Center for Building Technology. Pulse-Echo Ultrasonic Evaluation of the Integrity of Seams of Single-Ply Roofing Membranes: Results of Field Investigations and Recommenda-

H. Watanabe, and W. J. Rossiter. Nov 90, 42p NISTIR-4425

See also PB91-157172. Prepared in cooperation with Takenaka Corp., Tokyo (Japan). Technical Research Lab. Sponsored by Civil Engineering Lab. (Navy), Port Hueneme, CA.

Keywords: \*Ultrasonic tests, \*Roofing, \*Adhesive bonding, \*Seams(Joints), Nondestructive tests, Mechanical properties, Acoustic measurement, Construction materials, Roofs, Membranes, Inspection, Voids, Adhesion, \*Single-ply roofing membranes.

The report describes the second and final phase of a study to develop an ultrasonic NDE method for evaluating the integrity of seams of single-ply roofing mem-branes. The results of the laboratory evaluation of a prototype pulse-echo apparatus (the field scanner) were positive in that voids could be distinguished from were positive in that voids could be distinguished from well-bonded sections of the specimen using the intensity of the echo from the adhesive layer. In the Phase 2 study, seams of existing EPDM single-ply membranes were examined by roof-top scanning to evaluate the performance of the field scanner in practice. This was followed by laboratory tests to confirm and explain observations made during the field tests of the seams.

The field scanner was sensitive to micro-cavities, which could be generated in adhesive layers. This resulted in a number of 'false positive' readings. The formation of the micro-cavities was attributed to the temperature-induced volatilization of residual solvent remaining in the adhesive layer after its application on the membrane material.

100,111 PB91-162115 Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Chemical Engineering Science Div.

Automated High-Temperature Guarded-Hot-Plate Apparatus for Measuring Apparent Thermal Conductivity of Insulations between 300 and 750 K. Final rept.

J. G. Hust, B. J. Filla, J. A. Hurley, and D. R. Smith.

1990, 13p Contract ORNL/IA-21428 See also PB88-242060. Sponsored by Oak Ridge National Lab., TN.

Pub. in Insulation Materials, Testing, and Applications, ASTM STP 1030, p710-722 1990.

Keywords: \*Thermal insulation, \*Thermal conductivity, \*Test facilities, \*Thermocouples, Temperature meas-urement, Heat transmission, Algorithms, Heat transfer, Thermodynamic properties, Automatic control, Thermal measurements, Reprints.

An automated guarded-hot-plate apparatus was designed and built to meet the requirements of ASTM standard test method C 177 for measuring the thermal transmission properties of thermal insulation. The ap-paratus is controlled by a scientific desktop computer. Measurements with this apparatus can be performed at temperatures from 300 to 750 K in environments of different gases at pressures ranging from atmospheric pressure to roughig-pump vacuum. A novel design for a thermocouple device is used; this device more accurately senses the average temperature over the surface of each heater plate. An improved algorithm for the control sequence provides more stable heater powers and specimen temperatures. Initially the algorithm brings the system rapidly to a temperature set-point with minimal overshoot. It also permits highly sensitive control of the plate temperatures in later phases of the measurement sequence when thermal stability of the specimen boundaries is very important in measuring the thermal conductivity with high precision. Overall uncertainties of thermal conductivities at atmospheric pressure are 2% at 300 K and 3% at 750

100,112 PB91-162149 Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Center for Building Technology.

Computer Simulated Hydration of a Cement Model. Final rept.

Pub. in CIB.86 Proceedings, Washington, DC., September 22-26, 1986, v6 p2086-2095.

Keywords: \*Cements, \*Hydration, \*Microstructure, \*Cementing, Silicate cements, Computer simulation, Computer graphics, Bonding, Adhesion, Placing, Re-

A computer model is presented, which simulates the development of microstructure in hydrating tricalcium silicate paste. Hydration is programmed to proceed in steps, during which consumption of the anhydrous material occurs in increments and results in the produc-tion of calcium silicate hydrate and calcium hydroxide. Information concerning the distribution of the hydration products is processed by the program and is stored in computer files for later production of reports and two-dimensional representations of cross-sections of the simulated microstructure. These images can be compared to micrographs of polished samples of hydrated tricalcium silicate. The computer program permits the selection of the initial system parameters prior to the simulation, thus generating the microstructure under a variety of conditions.

PB91-167189 PC A05/MF A01 National Inst. of Standards and Technology (NCSL), Gaithersburg, MD. Review of Research Literature on Masonry Shear

C. W. C. Yancey, S. G. Fattal, and R. D. Dikkers. Feb 91, 100p NISTIR-4512

Portions of this document are illegible.

Keywords: \*Building codes, \*Masonry, \*Walls, Reviews, Design standards, Research, Standards, Loads(Forces), Compressive strength, Shear strength, Costruction.

A review of the technical literature on masonry shear wall tests was conducted to determine the range and depth of research conducted and to identify areas in need of additional research. The review covers docu-ments published from 1976 to 1989 and includes approximately seven hundred masonry wall tests. Both U.S. and foreign research was included in the review. U.S. code and standard requirements for the design of masonry shear walls are discussed and some of the provisions are highlighted in tabular and graphic form. Technical information regarding experimental studies is tabulated for easy reference and a selected number of test programs are examined in greater detail to present the objective and scope, test variables and major findings. Experimental data from comparable research studies are combined and analyzed to deter-mine the influence of key design parameters on the response of shear walls to in-plane lateral loading. Also included is a comparison of two experimentallyderived ultimate shear strength formulae with that included in the 1988 edition of the Uniform Building Code. The findings of the review are summarized and specific research needs are identified.

100.114

PB91-167197 PC A04/MF A01 Harvard Univ., Cambridge, MA. Div. of Applied Sciences

Ceiling Jet in Fires. Annual rept.

H. W. Emmons. Dec 90, 51p NIST/GCR-90/582 Grant NIST-60NANB8D0845

Sponsored by National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Center for Fire Re-

Keywords: \*Fires, \*Jet flow, \*Air flow, \*Ceilings(Architecture), Friction, Heat transfer, Entrainment, Fluid flow, Froude number, Buildings, Mathematical models.

The steady ceiling jet is examined with a simplified 'top heat' theory. Friction causes the jet to change downstream with flow, depth, and/or hydraulic jump adjustments to produce Richardson Number = 1 at the corridor exit, just as in hydraulics. Entrainment has a qualitative effect identical to friction, although there are quantitative differences. Heat transfer has, however, the opposite effect; the Richardson Number moves away from 1 as the flow proceeds. When all effects are included, high friction cases are predictable, while low friction cases are not. New experimental studies are needed to locate the reasons.

100.115

PB91-167304 PC A03/MF A01 PC A03/MF A01 National Inst. of Standards and Technology (BFRL), Gaithersburg, MD.

Computational Models Developed for the Corro-

sion of Prestressing Steel.
S. T. Wu, and J. R. Clifton. Mar 91, 20p NISTIR-4455
Prepared in cooperation with Air Force Office of Scientific Research, Bolling AFB, DC.

Keywords: \*Stress corrosion, \*Prestressing steels, \*Prestressed concrete, Fracturing, Fracture properties, Cracking(Fracturing), Reinforcing steels, Mathematical models, Structural steels, Fractures(Materials),

Modeling for the purpose of estimating the corrosion rates of steel in prestressed concrete are discussed in the paper. For steel in concrete, localized corrosion processes are not well understood. It is premature at present to develop a sophisticated but still incomplete mathematical model. Instead, a simplified approach is proposed for the quantitative evaluation of corrosion rates. A model was developed based upon consider-ations of diffusion processes and electrochemical reactions. The dominant chemical factors, such as the concentration of oxygen at the electrodes, are treated as primary variables in the differential equations. Two approaches which have been frequently used to treat stress corrosion cracking are briefly described. The first approach is based on a conventional engineering approach by estimating the stress intensity factors under various environments. In the second approach, the surface energy at grain boundaries is estimated along the crack path.

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100,116 PB91-167676 PC A03/MF A01 National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Center for Fire Research. Modern Test Methods for Flammability. V. Babrauskas. Jun 90, 25p NISTIR-4326

Keywords: \*Flammability testing, \*Fire tests, Combustion, Flames, Flammability, Calorimeters, Test facili-ties, Experimental data, Thermal measurements, Fires, Smoke, Ignition, Toxicity, Combustion products, Furniture, Corrosion, Heat transmission.

During the last decade, significant improvements have become available in flammability testing. Rationally-based new methods, derived from fundamental engi-neering principles are replacing the previously used empirical tests. The major emphasis in the development work has been to provide a basic set of bench-scale methods which can be used to predict full-scale product performance. Reference methods for conducting full-scale tests will continue to be needed to handle products or situations where the bench-scale methods are not applicable. The bulk of the testing needs, however, can now be fulfilled by use of benchscale tests which are not only simple to run, but are known to accurately predict the full-scale perform-

100,117 PB91-174573 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Fire Science and Engineering Div. Ceiling Jet-Driven Wall Flows in Compartment

Final rept.

L. Y. Cooper. 1988, 12p Pub. in Combustion Science and Technology 62, n4-6 p285-296 1988.

Keywords: \*Fires, \*Buildings, \*Compartments, \*Walls, Heat transfer, Plumes, Wall effects, Convection, Air flow, Combustion, Entrainment, Reprints.

Analytic estimates are developed for depth of penetration and lateral entrainment of negatively buoyant, ceiling jet-driven wall flows during early times of compartment fire scenarios. When walls are not too far from the fire source of the order of the fire-to-ceiling dis-tance, it is found that the penetration of these downward wall flows is a large fraction of the fire-to-ceiling distance, and that this fraction is relatively independent of the details of fire size and fire-to-wall spacing. Also, net rate of entrainment into the wall flow as it is buoyed back upward to the ceiling elevation is found to be several times larger than the flow rate of the driving ceiling jet flow immediately upstream of wall impingement. Data from five studies reported in the literature are reviewed relative to the anlytic results obtained. One of these involved a field model simulation of the flow generated by a buoyant source in an enclosure. Two experimental laboratory studies involved fires in enclosures with characteristic dimension of the order of several meters. Two others involved saltwater plumes in freshwater tanks with characteristic dimension of the order of several tenths of a meter. These data are found to be consistent generally with the analytic results, and, in particular, with the notion that the wall flows in question provide the mechanism for mixing which leads to the deep and rapid stratification typically observed in enclosed compartment fire environments

PB91-174789 Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Fire Safety Technology Div. Letter to the Editor of Standardization News.

Final rept.

Pub. in ASTM (American Society for Testing and Materials) Standardization News, p7-8 Feb 87.

Keywords: \*Fire tests, \*Standards, Research facilities, Measurement, Standardization, Metrology, Test facilities, Fires, Combustion, Reprints.

The letter to the editor responds to a short 'In My Opinion' article on the use, for regulatory purposes, of fire test methods designed for research and development (R&D).

100,119 PB91-175315 Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Building Materials Div.

Application of CCRL Data in the Development of Cement Standards. Final rept.

J. H. Pielert, and C. B. Spring, 1987, 12p Sponsored by American Society for Testing and Mate-rials, Philadelphia, PA.

Pub. in Uniformity of Cement Strength, ASTM STP 961, p30-41 1987

Keywords: \*Cements, \*Standards, \*Laboratories, Concretes, Quality assurance, Samples, Test facilities, Aggregates, Reinforcing steels, Portland cements, Construction materials, Reprints.

Cement and Concrete Reference Laboratory (CCRL) through its laboratory inspection and proficiency sample programs collects data which can be useful the development of cement and concrete standards. The paper outlines the scope of CCRL activities, discusses the nature of the CCRL data base, discusses specific examples of technical studies which support standard development, and outlines areas of future CCRL support to standards committees. CCRL inspections are conducted in laboratories equipped to perform tests on cement, concrete, concrete aggregate and steel reinforcing bars. The program for the distribution of proficiency samples includes portland cement, portland cement concrete, blended cement and masonry cement. Data from these programs have over the years been made available to the appropriate ASTM committees. CCRL also studies technical problems of interest to ASTM committees C1 and C9. Several CCRL activities will be presented to illustrate the application of CCRL data.

100,120 PB91-175422 Not available NTIS Mational Bureau of Standards (NEL), Gaithersburg, MD. Fire Measurement and Research Div. Smoke Production and Properties.

G. W. Mulholland. 1988, 10p Pub. in SFPE (Society of Fire Protection Engineers) Handbook of Fire Protection Engineering, Chapter 25, p368-377 1988.

Final rept.

Keywords: \*Smoke, \*Fires, \*Smoke detectors, Combustion products, Detectors, Transmittance, Visibility, Safety devices, Optical density, Safety engineering,

The fundamental concepts relevant to smoke are defined including smoke conversion factor, size distribution function, coagulation, light extinction coefficient, optical density, visibility, and smoke detector response function. Tabulated results are presented on smoke emission, average particle size and width of size distribution, specific optical density, and mass optical density for smoke produced by wood and plastics. Illustrative examples are included in regard to analyzing size distribution data, predicting the effect of particle coagulation on number concentration, estimating the visibility of an exit sign for a developing fire, and predicting smoke detector response time.

100,121 PB91-187278 Not available NTIS National Inst. of Standards and Technology (NEL),

Gaithersburg, MD. Building Environment Div.
Comparison of Two Test Methods for Determining
Transfer Function Coefficients for a Wall Using a Calibrated Hot Box. Final rept.

D. B. Burch, B. A. Licitra, and R. R. Zarr. 1990, 8p Sponsored by Department of Energy, Washington, DC. Pub. in Jnl. of Heat Transfer 112, n1 p35-42 Feb 90.

Keywords: \*Thermal measurements, \*Walls, \*Heat transfer coefficient, \*Temperature measuring instruments, Test facilities, Heat flux, Heat transmission, Heat transfer, Least squares method, Thermal analysis, Heat loss, Reprints.

The paper compares two dynamic test methods for obtaining empirical transfer-function coefficients (TFCs) for a wall specimen using a calibrated hot box (CHB). The wall specimen consisted of an insulated hollow concrete block wall that contained significant thermal bridges and lateral heat flows. The wall specimen was installed between the climatic and metering chambers of a CHB. The climatic chamber generated a dynamic (i.e., time-dependent) excitation function. The metering chamber maintained a typical indoor condition and served as a calorimeter. The transient heat-transfer rate at the inside surface of the wall specimen was determined at hourly time steps from an energy balance

of the metering chamber. The first method is called the 'curve fitting method.' In the method, a periodic excitation function consisting of a fundamental 24-hour sine wave and several harmonics (e.g., a sol-air diurnal temperature cycle) was generated in the climatic chamber. Empirical TFCs were obtained by curve fitting the measured specimen heat-transfer rate to a transfer function equation using the method of least squares.

100.122 PB91-187807 PC A04/MF A01 National Inst. of Standards and Technology (BFRL),

Gaithersburg, MD.

Building and Fire Research Laboratory Publications, 1990.

N. H. Jason. Apr 91, 69p NISTIR-4562 Also available from Supt. of Docs. See also PB90-

Keywords: \*Buildings, \*Fire safety, \*Bibliographies, Research management, Fire models, Fire tests,

Building and Fire Research Laboratory Publications, 1990 is the first edition to reflect the combined publica-tions of the Building and Fire Research Laboratory (BFRL) for calender year 1990. In 1991 the Center for Building Technology (CBT) and the Center for Fire Re-search (CFR) combined to form BFRL. The publication is a supplement to previous editions of Fire Research Publications and the Building Technology Publications.

100,123 PB91-189324 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Automated Production Technology Div.

Acoustic Technique for Evaluation of Thermal In-

Final rept.
D. R. Flynn, D. J. Evans, and T. W. Bartel. 1990, 24p
Pub. in Insulation, Materials, Testing, and Applications,
ASTM STP 1030, p319-342 1990.

Keywords: \*Thermal insulation, \*Noise(Sound), Frequencies, Fiberglass, Rock wool, Cellulose, Laboratory tests, Nondestructive tests, Sound transmission, ry tests, Reprints.

A laboratory apparatus has been constructed that enables rapid measurement of the sound insertion loss of a sample of insulation as a function of frequency. An extensive series of measurements of the sound insertion losses associated with blown samples of fiber-glass, rockwool, and cellulose has been completed; the results of these acoustic measurements are highly correlated with coverage (mass per unit area) and thermal resistance (R-value). An investigation is planned to extend the acoustic techniques used in the laboratory apparatus to in situ determination of the sound transmission loss through thermal insulation installed in attics. Two possible approaches to such field measurements are described.

Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Building Materials Div.

Field Testing of Adhesive-Bonded Seams of Rubber Roofing Membranes. Final rept.

W. J. Rossiter, J. F. Seiler, and P. E. Stutzman.

1989, 10p Pub. in Proceedings of Conference on Roofing Technology (9th), Gaithersburg, MD., May 4-5, 1989, p78-

Keywords: \*Adhesive bonding, \*Seams(Joints), \*Roofs, \*Rubber adhesives, Adhesion, Bonding, Me-\*Seams(Joints), Keywords: chanical properties, Dissimilar materials bonding, Membranes, Bonding strength, Construction materials,

Laboratory and field investigations were conducted to obtain data for supporting the development of a methodology to assure the quality of adhesive-bonded seams of vulcanized rubber membranes. The prime factors investigated were surface condition of the rubber, temperature of the rubber at the time of adhesive application and cure time of the adhesive. The laboratory data indicated that the T-peel test is sufficiently sensitive for use in a field methodology for assuring the quality of seams. Based on the laboratory results, it appeared possible to conduct the T-peel

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tests within a day (or perhaps less) of seam formation and to find significant differences in bond strength due to lack of proper surface cleaning of the rubber. Data from field applications are needed to demonstrate whether such differences are found on the job at one day's time or less. Seams sampled from two buildings were found to have low bond strengths, as compared to seams prepared using rubber carefully cleaned in the laboratory.

100,125 PB91-190124 PB91-190124 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Building Environment Div. Thermal Conductivity of Fumed Silica Board at Room Temperature.

Final rept. R. R. Zarr, and T. A. Somers. 1990, 13p Sponsored by Department of Energy, Washington, DC. Pub. in Thermal Conductivity 21, p247-259 1990.

ence Materials.

Keywords: \*Thermal insulation, \*Silicon dioxide, Thermal conductivity, US NIST, Reprints, Standard Refer-

The thermal conductivity of fumed-silica board insulation was measured using the 1-metre guarded hot plate at the National Institute of Standards and Technology (NIST). Measurements were conducted for the following ranges: bulk density, 304.5 to 325.4 kg/cu m; and air pressure, 97.51 to 103.43 kPa. The effect of moisture content on room-temperature measurements was minimized by prior conditioning of the specimen at 100C for 24 hours. A linear equation having two independent parameters, bulk density and air pressure, was fit to thirty-five data points. Certified values of ther mal resistance at room temperature were calculated mai resistance at room temperature were calculated for the following ranges of bulk density and air pressure; 300 to 330 kg/cu m and 97 to 102 kPa, respectively. The Office of Standard Reference Materials of NIST in Gaithersburg, Maryland, USA has made available two Standard Reference Materials (SRMs) of fumed-silica board, SRMs-1449 and 1459.

100,126 PB91-194696 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Building Environment Div.

Evaluation of the Heat Flux Transducer Technique for Measuring the Thermal Performance of Walls.

B. M. Burch, and R. R. Zarr. 1991, 11p Sponsored by Department of Energy, Washington, DC. Pub. in Proceedings of Conference on In-situ Heat Flux Measurements in Buildings Applications and Interpre-tations of Results, Hanover, NH., May 22-23, 1990,

Keywords: \*Heat flux, \*Thermal measurements, \*Walls, \*Energy conservation, Thermal analysis, Temperature distribution, Measuring instruments, Transducers, Heat transmission, Heat transfer, Temperature measurement, Reprints, \*Heat flux transducers.

Four wall specimens were instrumented with heat flux transducers and tested in a calibrated hot box to determine the accuracy of the heat flux transducers. The heat flux transducers were installed at the interior surface of the wall specimens and exposed to different steady and dynamic (i.e., time-dependent) temperature differences using a calibrated hox box. Two of the wall specimens were composed of homogeneous and monolithic material layers, which yielded virtually one-dimensional heat flux. The other two wall specimens were composed of conventional wall construction with wood structural members, which yielded a two-dimensional heat flux pattern. The heat flux transducers were previously calibrated by exposing them to a uniform heat flux in a guarded hot plate. The steady-state and transient heat flux transducer measurements agreed within 5% of the calibrated hot box measure-

100,127 PB91-203521 Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Building Materials Div.

NBS Research on Protective Coatings for Buildings and Structures.

Final rept.

L. W. Masters. 1985, 2p Pub. in Jnl. of Protective Coatings and Linings 2, n3 p15-16 Mar 85.

Keywords: \*Protective coatings, \*Structural steels, Research projects, Barrier coatings, Construction ma-

terials, US NBS, Performance prediction, Service life, Corrosion prevention, Weathering, Reprints.

The goal of coatings research in the Building Materials Division of the National Bureau of Standards (NBS) is to develop improved technical bases for assuring the quality of and for predicting the service life of protective coatings. The research results lead to test and evaluation methods and criteria to aid in the selection, use, and maintenance of protective coatings.

100,128 PB91-203935 Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Building Materials Div.
Use of Nondestructive Methods for Inspection of Single-Ply Roofing Membranes.

W. J. Rossiter, and J. R. Clifton. 1986, 10p Sponsored by Naval Civil Engineering Lab., Port Hueneme, CA.

Pub. in Durability of Building Materials 3, p343-352

Keywords: \*Nondestructive tests, \*Roofing, \*Membranes, Voids, Moisture content, Construction materials, Ultrasonic tests, Infrared thermography, Inspection, Roofs, Seams(Joints), Reprints.

The laboratory study investigated the use of the ultrasonic pulse echo method and the infrared thermo-graphy method to detect voids and delaminations non-destructively in seams of single-ply roofing membranes. Voids were intentionally incorporated in seam specimens prepared using a commercially available EPDM (ethylene-propylene-diene terpolymer) roofing membrane material. A number of factors affecting the response of the nondestructive evaluation (NDE) methods was examined, including: pressure applied during seam fabrication, void size, water in the void, temperature, unbonded seam interfaces, and supporting panel under the seam. The results indicated that both NDE methods were successful under certain laboratory conditions in locating hidden voids and delaminations in the seam specimens. Both the ultrasonic pulse echo and the infrared thermography methods need further research before their reliability in locating defects is ascertained and their results can be more fully interpreted.

100,129 PB91-206680 PC A04/MF A01 Factory Mutual Research Corp., Norwood, MA. Sprinkler/Hot Layer Interaction. Technical rept. Sept. 1990. G. Heskestad. May 91, 56p NIST/GCR-91/590 Grant NANB-OD1066 Sponsored by National Inst. of Standards and Technology (BFRL), Gaithersburg, MD.

Keywords: \*Fires, \*Sprinklers, \*Cooling, Vaporizing, Spraying, Evaporation, Entrainment, Interfaces, Fire protection, Spray quenching, Mathematical models, Temperature distribution, Boundary layer, Plumes.

A model has been developed for the cooling of a quiescent hot layer by a sprinkler spray in a two-layer zone model (with no direct interaction of the spray with a fire plume), based on existing models of spray-induced flow and heat transfer to evaporating drops. In addition, existing models have been adapted to predict the penetration of the spray-induced flow below the layer interface and associated entrainment of lower-layer fluid into the upper layer. The cooling model is in good agreement with published results from sprink-lered room-fire experiments, for which penetration of spray-induced flow into the lower layer and associated entrainment were calculated to be negligible. No published results have been found to test the validity of the adapted models of penetration and associated entrainment, which do not account for possible effects of the spray below the layer interface.

PB91-216648 PC A04/MF A01
National Inst. of Standards and Technology (NEL),
Gaithersburg, MD. Robot Systems Div.
Description of a Vibration Compensation System
for the Small Scale Model Robot Crane Project.
R. Bostelman. Jul 91, 70p NISTIR-4595 100,130 PB91-216648

\*Cranes(Hoists), \*Robotics, Keywords: damping, Construction equipment, Models, Computer systems hardware, Electronics, Design, Data acquisition, Control systems, Systems engineering, Circuit diagrams, Servo control, SSMRC(Small Scale Model Robot Crane).

The report describes the electronic hardware designed and developed for the Small Scale Model Robot Crane (SSMRC) Project sponsored by the Defense Advanced Research Projects Agency (DARPA). The purpose of the electronic hardware is to provide the necessary servo controls for the three axes of the SSMRC. The report begins with an introduction which explains the overall objectives of the project and describes the SSMRC system configuration. An electronic design section discusses each system component and describes the component from both a hardware and a system point of view. Test procedures and re-sults, which give the troubleshooting methods and data needed for development of the system, are then presented. The report concludes with a brief summary and an appendix which provides electronic design schematics and descriptions of the parts used in the construction of the electronic hardware system.

100.131

PB91-216689 PC A05/MF A01 National Inst. of Standards and Technology (BFRL), Gaithersburg, MD.

Applications of the Generalized Global Equivalence Ratio Model (GGERM) for Predicting the Generation Rate and Distribution of Products of Combustion in Two-Layer Fire Environments: Methane and Hexanes.

L. Y. Cooper. Jun 91, 78p NISTIR-4590

Keywords: \*Combustion, \*Fires, \*Buildings, \*Methan, \*Hexane, Combustion products, Reaction kinetics, Mathematical models, Fluid flow, Chemical reactions, Steady state.

The Generalized Global Equivalence Ratio Model (GGERM) was developed to predict the generation rates of oxygen, fuel, and other products of combustion in rooms containing fires. The GGERM extends to general transient conditions the global equivalence ratio model established during times of steady-state in experimental studies involving two-layer compartment fires. The present work uses the GGERM to predict upper layer mass fractions of products of combustion (fuel, oxygen, CO, and others) in these two-layer fire experiments, but during times of transient response. All predicted results are found to be plausible and, where transient data are available, predicted and measured results compare favorably. However, available data are limited and additional validation of the GGERM under more varied fire conditions is required before it can be used with confidence in two-layer zone-type compartment fire models.

100,132

PB91-216788 PC A08/MF A02 National Inst. of Standards and Technology (BFRL), Gaithersburg, MD.

Building and Fire Research Project Summaries,

N. J. Raufaste. Jun 91, 155p NISTIR-4582 See also PB91-187807.

Keywords: \*Research projects, \*Fires, \*Buildings, Flammability, Fire resistant materials, Combustion, Fire safety, Indoor air quality, Fire hazards, Smoke, Fire protection, \*Building and Fire Research Laborato-

In early 1991, as part of an agency-wide reorganization, the National Institute of Standards and Technology (NIST) created the Building and Fire Research Lab-oratory (BFRL) by merging its Centers for Building Technology and Fire Research. BFRL's mission is to increase the usefulness, safety, and economy of constructed facilities, and reduce the human and economic costs of unwanted fires in buildings. The report sum-marizes BFRL's research for 1991. The report is arranged by its research programs: structural engineering, materials engineering, mechanical and environ-mental systems, fire science and engineering, and fire measurement and research. Each summary lists the project title, its research, the BFRL point of contact, sponsor, and results.

100,133

PB91-237479 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Building Materials Div.

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Microstructural Aspects of the Fracture of Hardened Cement Paste.

Final rept. L. Struble, P. Stutzman, and E. Fuller. 1989, 5p Contract AFOSR-ISSA88-0039

Sponsored by Air Force Office of Scientific Research, Bolling AFB, DC.

Pub. in Jnl. of the American Chemical Society 72, n12 p2295-2299 1989.

Keywords: \*Fracture mechanics, \*Cements, \*Crack propagation, Microstructure, Paste(Consistency), Hardness, Electron microscopy, Microcracks, Construction materials. Reprints.

Microstructures of fractured hardened cement pastes were examined using a scanning electron microscope. Cracks generally appear to pass around unhydrated cement grains and along calcium hydroxide cleavage planes, but to pass through voids, inner hydration product, and outer hydration product with no change in direction. The crack path is often offset, with gaps between offset segments forming bridges. The crack is often branched or forked at the tip, and microcracks are observed just ahead of the tip. The gaps between crack offsets may explain the rising fracture resistance (R-curve) of hardened cement paste, and the micro-cracking ahead of the crack tip may also provide toughening.

100,134 PB92-108919 PC A03/MF A01 National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Center for Fire Research. FPETOOL User's Gulde.
H. E. Nelson. Oct 90, 38p NISTIR-4439
Contract GSA/PBS-87-03

Sponsored by Public Buildings Service, Washington, DC.

Keywords: \*Fire hazards, \*Fire protection, \*Computer applications, Computerized simulation, Buildings, Mathematical models, Fire safety, Smoke, Flame propagation, Sprinkler systems, Fire detection systems, Ventilation, Flashover, User manuals (Computer programs), \*FPETOOL computer program.

FPETOOL is a computerized package of relatively simple engineering equations and models. FPETOOL consists of a package of engineering tools useful in estimating potential fire hazard and the response of the space and fire protection systems to the developing hazard. To a large extent, user instructions are included as screen messages presented at the time of need by FPETOOL. The document covers information useful to the user, but not included as screen messages.

100,135 PB92-108976 PC A03/MF A01 National Inst. of Standards and Technology (BFRL), Gaithersburg, MD. Mathematical Modeling of Enclosure Fires. H. E. Mitler. May 91, 47p NISTIR-90-4294 See also PB90-129867 and PB81-110520.

Keywords: \*Fires, \*Mathematical models, \*Enclosures, Fire hazards, Fire safety, Fire tests, Combustion, \*Fire models, Field models, Zone models.

After a brief description of the history and physics of enclosure fire modeling, two kinds of deterministic fire models are discussed: field models and zone models. The models consist of sets of coupled equations -- dif-ferential, algebraic, or a mixture of the two. Special emphasis is placed on discussing some of the numerical techniques used to solve these equations. Although this is not a comprehensive review article, an attempt has been made to give a sufficiently complete reference section that the interested reader can follow up on any item.

100,136 PB92-112556 PC A03/MF A01 California Univ., Berkeley. Dept. of Mechanical Engi-

Users' Guide to BREAK1, the Berkeley Algorithm for Breaking Window Glass in a Compartment Fire. A. A. Joshi, and P. J. Pagni. Oct 91, 29p NIST/GCR-91/596

Grant NANB-80848

See also PB90-244443 and PB88-111810. Sponsored by National Inst. of Standards and Technology (BFRL), Gaithersburg, MD.

Keywords: \*Fires, \*Buildings, \*Window glass, \*Break-\*Computer applications, Mathematical models, Thermal stresses, Thermal conductivity, Thermal diffusivity, Thermal expansion, Absorption, Modulus of elasticity, Temperature, Heat transfer coefficient, Emissivity, Flames, Radiation, Thermophysical properties, Vents, User manuals(Computer programs)

The report is an instructional manual for the computer program BREAK1, the Berkeley Algorithm for Breaking Window Glass in a Compartment Fire, version 1.0. The thermal response of window glass exposed to a com-partment fire and its time to breakage are calculated. The following glass properties, treated here as constant, are required as input: thermal conductivity, thermal diffusivity, absorption length, breaking stress, Young's modulus, coefficient of linear thermal expansion and emissivity. In addition, the ambient tempera-ture, the hot layer temperature, heat transfer coeffi-cients and emissivities and the direct flame radiation histories are needed as input. The window geometry is also required. The output describes the evolution of the window temperature field, T(x,t), where x is the direction normal to the glass pane, culminating in the window breakage time, t sub(b). The manual contains a summary of the mathematical model, sample thermophysical and mechanical data tables, some worked examples and advice on using the program.

PB92-116334 PC A04/MF A01 National Inst. of Standards and Technology, Gaithersburg, MD.

Analysis of Moisture Accumulation in a Wood

Frame Wall Subjected to Winter Climate.
D. M. Burch, and W. C. Thomas. Oct 91, 57p

NISTIR-4674

See also DE90014155 and PB85-199248. Sponsored by Department of Energy, Washington, DC.

Keywords: \*Moisture content, \*Walls, \*Construction materials, \*Wood products, Framed structures, Sheathing, Humidity, Heat transfer, Mathematical models, Permeability, Finite difference method, Thermal insulation. Winter mal insulation, Winter.

A transient, one-dimensional, finite-difference model is presented that predicts the coupled transfer of heat and moisture in a multilayer wall under nonisothermal conditions. The model can predict moisture transfer in the diffusion through the capillary flow regimes. It has a provision to account for convective moisture transfer by including embedded cavities which may be coupled to indoor and outdoor air. The model is subsequently used to predict the time-varying average moisture content in the sheathing and siding of a wood frame wall as a function of time of year. Results are shown for a mild winter climate (Atlanta, GA), an intermediate winter climate (Boston, MA), and a cold winter climate (Madison, WI). The indoor temperature is maintained at 21 C, and separate computer runs are carried out for indoor relative humidities of 35% and 50%. The effect of several construction parameters on the winter moisture accumulation are investigated. The parameters include the interior vapor retarder permeance, sheathing permeance, exterior paint permeance, indoor air leak age, and the amount of insulation.

100.138 PB92-116342 PC A03/MF A01 National Inst. of Standards and Technology (NCSL), Gaithersburg, MD. Ultimate Strength of Masonry Shear Walls: Predic-

tions versus Test Results. S. G. Fattal, and D. R. Todd. Oct 91, 47p NISTIR-

See also PB91-167189.

Keywords: \*Ultimate strength, \*Masonry, \*Walls, Shear stress, Building codes, Loads(Forces), Mathematical models, Design standards, Earthquake resistant structures, Structural analysis, Earthquake engi-

The study compares the ability of four different equations to predict the ultimate shear stress in masonry walls failing in shear. Experimental data on full-grouted reinforced shear walls from four different sources are compared with the predictions from the four equations. Wall characteristics from 65 test specimens were used as input to the four predictive equations. The ultimate strength predictions were then compared to the actual measured strength of the 65 test walls. Two of the equations (the existing UBC equation for shear strength of masonry walls and the Architectural Institute of Japan's equation for predicting the shear strength of reinforced concrete shear walls) were found to be inadequate for the prediction of ultimate shear strength of masonry walls. An equation proposed by Shing et al. was found to predict shear strength well for only limited ranges of variables, primarily because excessive weight is given to the contributions of horizontal reinforcement to strength. An equation proposed by Matsumura was found to be the best predictor of the four equations examined, but it lacks the consistency needed to use it as a basis for

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PB92-116458 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Fire Measurement and Research PB92-116458

Large-Scale Validation of Bench-Scale Fire Toxicltv Tests.

Final rept

V. Babrauskas, R. H. Harris, E. Braun, B. C. Levin, M. Paabo, and R. G. Gann. 1991, 24p Pub. in Jnl. of Fire Sciences 9, n2 p125-148 Mar/Apr

Keywords: \*Fire tests, \*Standards, \*Toxicity, \*Construction materials, Test methods, Fire hazards, Test facilities, Chemical properties, Proving, Bench-scale experiments, Buildings, Reprints.

A sizable number of bench-scale fire toxicity tests have been proposed over the last two decades. To date, no test method has successfully passed through the standards bodies ISO, ASTM, or BSI. The reasons are varied, but a major concern has been that none of the methods were seen to adequately predict the be-havior of real, large-scale building fires. Such valida-tion efforts have been held back both due to a shortage of good quality data, and because agreement had not been reached on the criteria for successful validation. NIST has now completed a pilot project to address both of these issues. In the study, several criteria for validation have been put forth. An initial data set has been compared against these criteria, comprising 2 bench-scale methods, 3 test materials, and a single real-scale fire scenario. The project results indicate that the course being pursued is appropriate, and pro-vide illustrative performance data for the two bench-scale methods. The present project was a pilot study; further validation data will have to come from additional test materials and additional real-scale fire scenarios being examined. As a result of the studies, a factorof-3 agreement between bench-scale and real-scale results was established as both useful and practical.

100.140 PB92-116557 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Structures Div. Impact-Echo: A New Method for Inspecting Construction Materials.

Final rept. N. J. Carino, and M. Sansalone. 1990, 15p in Nondestructive Testing and Evaluation for Manufacturing and Construction, p209-223 1990.

Keywords: \*Construction materials, \*Nondestructive keywords: "Construction materials, "Nondestructive tests, "Concretes, Impact tests, Fourier transformation, Stress waves, Measurement, Displacement, Frequency response testing, Surface properties, Reflection, S waves, P waves, Transducers, Frequency, Spectrum analysis, Graphic methods, Cross-sections, Voids, Wave propagation, Delaminating, Defects, Reprints, \*Impact echo technique.

A technique called impact-echo has been developed for flaw detection in heterogenous construction materials such as concrete. The technique, which is based on a simple concept, uses mechanical impact to generate a short duration stress pulse which travels into the test object as P- and S-waves. The waves are reflected by internal discontinuities or by external boundaries. A displacement transducer located close to the impact point monitors the dynamic surface displacement caused by the arrival of the reflected waves. The stress waves propagate back and forth between the test surface and an internal discontinuity (or external surfaces). Thus, a transient resonance condition is created, and the displacement waveform has a periodicity which is dependent on the P-wave speed and the distance between the reflecting surfaces. The periodicity was a periodicity which is dependent on the P-wave speed and the distance between the reflecting surfaces. The periodicity was a periodicity which is the periodicity with the periodicity was a periodicity with the periodicity was a periodicity which is the periodic which is the periodic which is the periodic which is the periodicity which is the periodicity which is the periodicity which is the periodic which is th dicity is determined by using the fast Fourier transform to obtain the dominant frequency in the waveform. Knowing the P-wave speed, the frequency value is used to compute the distance from the surface to the reflecting interface. The paper discusses the theoretical basis of the method and summarizes laboratory

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and field studies, which illustrate the capabilities of the technique. A data analysis technique, called spectral peak plotting, is described.

100.141

PB92-116821 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Building Materials Div. Integrated Knowledge Systems for Concrete Sci-

ence and Technology.

Final rept.

G. Frohnsdorff. 1989, 18p See also PB89-176119.

Pub. in Materials Science of Concrete I, p315-332

1989

Keywords: \*Concretes, \*Data bases, \*Artificial intelligence, \*Expert systems, \*Cements, Mathematical models, Software engineering, Knowledge models, Software engineering, bases(Artificial intelligence), Reprints.

The rapid changes in ability to process, store, and retrieve knowledge brought about by advances in computers and telecommunications have enormous implications for concrete science and technology. Knowledge stored in computers will take on new dimensions as society's collective memory of concrete science and technology grows into a more integrated body of knowledge than has previously been possible. It will make possible powerful decision support systems and will raise problems about the sharing of knowledge. Integrated knowledge systems will consist of text bases, databases, model bases, rule bases, and image bases which may be interfaced through computer networks. It is to be expected that some or all of these forms of knowledge base will become standardized through the voluntary consensus standards process. Development of the integrated knowledge systems will draw attention to the gaps in knowledge and should lead to collaboration between researchers in planning research to fill the gaps. For the systems to develop most effectively, protocols for developing and interfacing the subsystems will need to be developed. The benefits of collaboration will be predictive tools with a power which far exceeds that of anything presently available.

100,142

PB92-123033 PC A07/MF A02 National Inst. of Standards and Technology (BFRL), Gaithersburg, MD.
Flammability Characterization of Foam Plastics.

T. G. Cleary, and J. G. Quintiere. Oct 91, 143p NISTIR-4664

Sponsored by Society of the Plastics Industry, Washington, DC.

Keywords: \*Flammability, \*Polyurethane foam, Ignition, Flammability testing, Flame propagation, Test methods, Test facilities, Standards, Flame calorimeters, Heat measurement, Fire resistance, Constructives. tion materials, Polystyrene, Plastics, ASTM E-84 test.

The results of a study to identify an alternative test protocol to the ASTM E-84 (Steiner Tunnel) test as a measure of flammability for foamed plastics are presented. New fire test apparatuses, namely, the Cone Calorimeter and the Lateral Ignition and Flame Spread apparatus were used to more completely characterize foamed plastic flammability. Key flammability properties obtained from these apparatuses describe ignit-ability, flame spread rate, rate of heat release, and smoke obscuration. An extensive data set of these flammability properties for 10 selected foamed plastics was generated. The tested materials included melting foams (polystyrene foams) and charring foams (polyurethanes, polyisocyanurate and phenolic foams). The effects of melting and dripping were limited by testing the materials in the horizontal orientation. In addition, an integrated approach to material flammability characterization is presented that uses these parameters to predict fire growth potential.

#### Structural Analyses

100,143

PB91-134668 Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Structures Div.

Preliminary Dynamic Analyses of the Ministry of Agriculturé Building. Final rept.

W. C. Stone, and N. R. Cuevas. 1986, 22p

Pub. in Proceedings of International Conference on Mexico Earthquakes - 1985: Factors Involved and Lessons Learned, Mexico City, Mexico, September 19-21, 1986, p233-254.

Keywords: \*Earthquake resistant structures, \*Dynamic structural analysis, \*Public buildings, \*Concrete structures, Model tests, Mexico City, Concrete slabs, Concrete construction, Reinforced concrete, Seismic waves, Reprints, \*Structural vibration, Earthquake enaineering. Finite element method.

The Ministry of Agriculture Building on Avenida San Antonio Abad (Mexico City) was originally constructed as a 17-story reinforced concrete waffle slab system with interior reinforced concrete shear walls surrounding the elevator shafts and stairwells. The plan was assymetrical and included an attached laterally braced annex which protruded from the southwest side of the building. During the 1985 Mexico earthquake it suffered significant damage but did not collapse. Rehabilitation plans for the structure are discussed as well as free vibration tests conducted in the post-earthquake configuration. A structural model of the building was prepared as part of a preliminary investigation on its dynamic behavior during the 1985 earthquake. The model was developed using three dimensional finite elements as part of a benchmark study to determine the feasibility of this analytical approach. Observations on the computational burden and difficulty of employing such detailed computer models are discussed.

PC A03/MF A01 PB91-167239 National Inst. of Standards and Technology (BFRL),

Gaithersburg, MD.
Measurement of Structural Response Characteristics of Full-Scale Buildings: Selection of Struc-

tures. R. D. Marshall, L. T. Phan, and M. Celebi. Feb 91, 22p NISTIR-4511

Prepared in cooperation with Geological Survey, Menlo Park, CA. Branch of Engineering Seismology and Geology.

Keywords: \*Structural vibration, \*Buildings, \*Dynamic response, \*Measurement, \*Earthquake engineering, Structural engineering, Earthquakes, Field tests, Dynamic structural analysis, Measuring instruments, Seismic waves, Loma Prieta Earthquake.

The report describes the selection of existing building structures for subsequent field measurements of lowlevel ambient vibrations. By comparing measurement results with previously recorded high-level responses, it is anticipated that guidance can be developed for improved measurement practice. The buildings selected for the effort represent a cross-section of contemporary structural systems and materials, foundation types, and a range of building heights and aspect ratios. Each building was subjected to strong shaking during the Loma Prieta Earthquake of October 17, 1989

PB91-184846 PC A14/MF A02 National Inst. of Standards and Technology (BFRL), Gaithersburg, MD.

Proceedings of a Workshop on Evaluation, Repair, and Retrofit of Structures. U.S.-Japan Panel on Wind and Seismic Effects, UJNR. Held in Gaithers-

burg, MD., USA, on May 12-14, 1990. J. O. Jirsa. Apr 91, 305p NISTIR-4515

Prepared in cooperation with Texas Univ. at Austin. Sponsored by National Science Foundation, Washington, DC.

Keywords: \*Earthquake engineering, Structural analysis, \*Earthquake resistant structures, Earthquake damage, Retrofitting, Repair, Concrete structures, Steel structures, Reinforced concrete, Structural members, Seismic waves, Wind effects.

The report is the Proceedings of an international workshop on Evaluation, Repair, and Retrofit of Structures. The workshop was a joint effort of Task Committees C and D, 'Repair and Retrofit of Existing Structures' and 'Evaluation of Structural Performance' respectively of the U.S.-JAPAN Panel on Wind and Seismic Effects. The workshop was hosted by the National Institute of Standards and Technology during May 12-14 1990. The National Science Foundation provided the financial support. The subjects addressed included: evaluation of structures; performance of existing structures their repair and strengthening; and research on techniques for repairing and retrofitting structures.

100,146

PB91-204057 Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Structures Div.

Investigation of the Collapse of L'Ambiance Plaza.

Final rept. C. F. Scribner, and C. G. Culver. 1988, 22p Pub. in Jnl. of Performance of Constructed Facilities 2, n2 p58-79 May 88.

Keywords: \*Accident investigations, \*Lift slab construction, \*Collapse, \*Buildings, Failure, Concrete slabs, Loads(Forces), Concrete structures, Concrete construction, Structural members, Structural analysis, Reprints.

Results from an investigation of the collapse of the L'Ambiance Plaza building on April 23, 1987, are pre-sented. The building was being constructed using the lift-slab method; collapse occurred during construc-tion. The investigation included examination of debris at the site of the collapse, review of eyewitness accounts of the collapse, review of project documentation, laboratory and field tests and analyses of the structure. Several potential failure mechanisms were investigated. The most probable cause of the collapse was determined to be loss of support by a lifting jack in the west tower during placement of a group of three floor slabs. The loss of support was likely due to excessive deformation of a shearhead lifting angle which caused a lifting nut to slip off the lifting angle of the shearhead. The failure mechanism was duplicated in laboratory experiments. As loads were redistributed after the initial failure, the remaining jack rods along column line E supporting the package of floor slabs slipped off the lifting angles and the slabs failed in flexure and shear. These slabs fell, causing the slabs below them to fail.

100.147

PB91-204206 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Center for Building Technology. Research and Technology for Structural Engineer-

ing Productivity. Final rept.

R. N. Wright. 1991, 7p

Sponsored by American Society of Civil Engineers, New York.

Pub. in Proceedings of Structures Congress, Indianapolis, IN., April 29-May 1, 1991, p1-7.

Keywords: \*Structural engineering, \*Productivity, Competition, Research, Structural design, Construc-\*Productivity, tion, Artificial intelligence, Automation, Robotics, Safety, Civil engineering, Reprints.

Structural engineers strive to shelter and support human activities with safe, functional, economic and esthetic structures. Engineers' productivity is measured by the value of their results and the efficiency with which their results are obtained. Demands for improved structural engineering services include: reducing vulnerability to natural disasters, conserving and renewing existing structures, building on difficult sites, protecting the environment, conserving scarce re-sources, and creating structural systems consistent with evolving human aspirations. Structural engineers will be challenged by colleagues abroad to maintain leadership and competitiveness in structural engineer-ing practice in an increasingly international construcmarketplace, and by other professions which may take advantage of their growing knowledge and advanced technologies to extend their activities into what variced technicingles to extend their activities into whise is now structural engineering practice. Productivity, value to the customer, should be the deciding factor. Technical leadership is key to the productivity and vitality of structural engineering. Emerging technologies, such as advanced materials, artificial intelligence, automated to be the contractivities and the tractions and the tractions are the contractivities. tomation and robotics, can greatly increase the powers of structural engineers. Strong research, development and educational efforts are needed to adapt and exploit emerging technologies.

100.148

PB91-206714 PC A03/MF A01 National Inst. of Standards and Technology (BFRL), Gaithersburg, MD.

#### Structural Analyses

Long Term Performance of Rubber in Seismic and Non-Seismic Bearings: A Literature Review.
J. W. Martin. Jun 91, 30p NISTIR-4613

Keywords: \*Vibration insulators, \*Rubber, \*Bearings, Earthquake resistant structures, Vibration damping, Structural vibration, Seismic waves, Service life, Reviews, Earthquake engineering, Loads(Forces).

The use of seismic isolation bearings to decouple buildings and lifeline structures from strong ground motion has received an increased amount of attention in recent years. While several types of seismic isolator bearings have been developed and proposed for use, the most common type is the laminated rubber (elastomeric) bearing. Because the design lifetime of these bearings is expected to be on the order of 50 to 100 years, the long-term performance of the rubber (elastomer) must be addressed. Therefore, a literature review was conducted to identify potential limits on the long-term performance of rubbers (elastomers) used in bearings. Several issues, including the need for con-sensus of performance standards and for additional research on the effects of creep, aging, temperature, and high-energy radiation on the properties of rubber.

100 149

PB91-222570 PC A05/MF A01 National Inst. of Standards and Technology (NEL), Gaithersburg, MD.

Performance of 1/3-Scale Model Precast Concrete Beam-Column Connections Subjected to Cyclic In-

elastic Loads. Report No. 2. G. S. Cheok, and H. S. Lew. Jun 91, 85p NISTIR-

See also PB91-107623.

Keywords: \*Cyclic loads, \*Earthquake resistant structures, \*Beams(Supports), \*Precast concrete, \*Construction joints, Concrete structures, Concrete construction, Earthquake engineering, Model tests, Ductility, Failure.

Results are presented from the experimental test program on precast concrete beam-column connections subjected to inelastic cyclic loads being conducted at the National Institute of Standards and Technology. The report is the second in a series and covers the test results from Phase II of a three phase program. The objective of the test program is to develop an economical moment resistant precast beam-column joint for high seismic zones. Test specimens are 1/3-scale models of a prototype interior concrete beam-column connection. The 1985 UBC design criteria for seismic Zones 2 and 4 were used. Six specimens were tested. The experimental variables include the location of the post-tensioning force and the type of post-tensioning tendons used. Comparisons of the performance among these specimens are made. Comparisons with the monolithic specimens are also presented. These comparisons are made based on the failure mode, energy absorption characteristics, strength and ductility of the connection.

PB91-236588 Not available NTIS National Inst. of Standards and Technology (BFRL), Gaithersburg, MD. Structures Div.
Performance of Precast Concrete Beam-to-

Column Connections Subject to Cyclic Loading. Final rept.

Pub. in PCI (Prestressed Concrete Institute) Jnl. 36, n3 p56-67 May/Jun 91.

Keywords: \*Precast concrete, \*Cyclic Beams(Supports), \*Columns(Supports), \*Concestors, Earthquake resistant structures, Loads(Forces), Concrete construction, brombers Buildings, Re-

An experimental study of the behavior of precast concrete beam-to-column connections subjected to cyclic inelastic loading conducted at the National Institute of Standards and Technology is presented. The study was initiated to provide data for the development of a rational design procedure for such connections in seis-mically active regions. The objective of the study is to develop a moment resistant precast concrete connection that is economical and can be easily constructed. Four one-third scale monolithic concrete beam-tocolumn connections were tested: two were designed according to the 1985 Uniform Building Code (UBC) Seismic Zone 2 criteria and two to UBC Zone 4 criteria. In addition, two precast, past-tensioned concrete

beam-to-column connections similar in design to the monolithic Zone 4 specimens were tested. These tests constitute the first phase of a multi-year test program.

PB91-237834 Not available NTIS National Inst. of Standards and Technology (BFRL), Gaithersburg, MD. Building and Fire Research Lab

Assessment: U.S. Office Building of Moscow.

R. N. Wright, N. J. Carino, J. G. Gross, and M. Sansalone. 1989, 14p Pub. in Jnl. of Performance of Constructed Facilities 3, n1 p2-15 Feb 89.

Keywords: \*Buildings, \*Structural analysis, \*Damage assessment, Inspection, Construction, Structural members, Masonry, Steels, Concretes, Deterioration, Construction materials, Office buildings, \*US Embassy(Moscow).

On October 30, 1986, the United States Congress directed the National Bureau of Standards (NBS) to conduct an independent analysis of the new United States Embassy Office Building being constructed in Moscow. The analysis was to include '...an assessment of the current structure and recommendations and cost estimates for correcting any structural flaws and construction defect....' The paper describes the history of the building project, the site and building, and the process of investigation, which included field, laboratory and analytical studies, and its findings. The investigation identified important structural defects in the vestigation the time time time to the total structural defects in them. While important, these structural defects, in comparison to the total structural system, are modest in scale and fully correctable. Companion papers describe the assessments of: the structural system, the masonry enclosure, and the potential for progressive collapse.

PB92-116425 PC A99/MF A06 National Inst. of Standards and Technology (BFRL),

Gaithersburg, MD.
Wind and Seismic Effects. Proceedings of the Joint Meeting of the U.S.-Japan Cooperative Pro-gram in Natural Resources Panel on Wind and Seismic Effects (23rd). Held in Tsukuba, Japan, on May 14-17, 1991.

May 14-17, 1991.
Special pub. (Final).
N. J. Raufaste. Sep 91, 639p NIST/SP-820
Also available from Supt. of Docs. as SN003-003-03107-1. See also DE91005427 and PB91-107094.

Keywords: \*Wind pressure, \*Earthquakes, quake resistant structures, Highway bridges, Buildings, Dynamic structural analysis, Dynamic loads, Dams, Building codes, Structural design, International cooperation, Wind loads.

The publication is the proceedings of the 23rd Joint Meeting of the U.S.-Japan Panel on Wind and Seismic Effects. The meeting was held at the Public Works Research Institute, Tsukuba, Japan, during May 14-17, 1991. The proceedings include the program, list of 1991. The proceedings include the program, list of members, panel resolutions, task committee reports, and 42 technical papers. The papers were presented under seven themes: (1) Wind Engineering; (2) Earthquake Engineering; (3) Storm Surge and Tsunamis; (4) Joint Cooperative Research Program; (5) Performance of Nonstructural Systems; (6) International Decade for Natural Disaster Reduction; and (7) Summaries of Task Committee Workshop Reports.

#### General

100.153 PB91-149302 Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research. Application of Fire Research.

J. E. Snell. 1986, 20p Pub. in Proceedings of International Meeting of Fire Research and Test Centers, Avila, Spain, October 7-9, 1986, p97-116.

Keywords: Methodology, Technology transfer, Fire tests, Performance tests, Fire safety, Test facilities,

Research management, Reprints, \*Center for Fire Research, \*Fire research.

The role of the Center for Fire Research is discussed with three examples of recent major projects. It is predicted that the methodology being developed will lead toward performance codes for fire safety.

100,154 PB91-159764 PC A04/MF A01 National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Center for Computing and Applied

NIST 'Building Life-Cycle Cost' (BLCC) Program (Version 3.0). User's Guide and Reference Manual. S. R. Petersen, Jan 91, 54p NISTIR-4481

Sponsored by Department of Energy, Washington, DC. Federal Energy Management Program Staff.

Keywords: \*Buildings, \*Economic analysis, \*Benefit cost analysis, \*Computer applications, Return on investment, Operating costs, Energy conservation, Projects, Savings, Program evaluation, User manuals(Computer programs), Building Life-Cycle Cost computer program, National Institute of Standard and Parkers (Programs). ards and Technology.

The NIST Building Life-Cycle Cost (BLCC) computer program provides economic analysis of proposed capital investments that are expected to reduce long-term operating costs of buildings or building systems. It is especially useful for evaluating the costs and benefits of energy conservation projects in buildings. Two or more alternative designs can be evaluated to deter-mine which has the lowest life-cycle cost. Economic measures, including net savings, savings-to-invest-ment ratio, and adjusted internal rate of return, can be calculated for any design alternative relative to the designated base case. BLCC can be used for evaluating both Federal and private sector projects. It complies with ASTM standards related to building economics as well as FEMP and OMB A-94 guidelines for economic analysis of Federal building projects. BLCC is designed to run on an IBM-PC or compatible microcomputer with approximately 640K of random access memory, with or without a hard disk.

100.155 PB91-167254 PC A03/MF A01 National Inst. of Standards and Technology (BFRL), Gaithersburg, MD. **Experimental Study of Top Vented Compartment** 

K. M. Tu. Feb 91, 34p NISTIR-4499

Keywords: \*Fires, Room fires, Ventilation, Tests, Ceilings(Architecture), Models, Flow rate, Differential pressure, Vents.

In a top vented compartment fire, both density difference and pressure difference across the horizontal ceiling vent control the vent flow. The research work pursued experimental studies and investigations of exchange flows through a horizontal ceiling vent as related to solely top vented compartment fire situations. A cubic box with inside dimensions of 0.43  $\times$  0.43  $\times$  0.43 m high (17 x 17 x 17 in) and walls of 0.025 m (1 in) thick Kaowool was employed for the compartment fire tests. For compartment fires of various horizontal ceiling vent sizes: (1) the fuel mass burning rates were measured, and (2) the air and combustion-flue-gas exchange flow rates were estimated based on (i) available theories and (ii) gas concentrations in the fire compartment.

100.156 PC A06/MF A01 PB91-167270 National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Center for Fire Research. Role of Bench-Scale Test Data In Assessing Real-Scale Fire Toxicity.

Technical note (Final).
V. Babrauskas, R. H. Harris, E. Braun, B. Levin, M. Paabo, and R. G. Gann. Jan 91, 113p NIST/TN-

Also available from Supt. of Docs.

Keywords: \*Fires, \*Toxicology, Furniture, Room fires, Lethality, Laboratory animals, Polyurethane resins, Polyvinylchloride, Gases, Bench-scale experiments.

The need was seen for establishing a methodology by which bench-scale fire toxicity methods could be validated against real-scale room fires. The present study is the result of a pilot project in the area. Appropriate

General

validation hypotheses have been put forth and examined in the context of some initial data. Three materials - Douglas fir, rigid polyurethane foam, and PVC - were examined in real-scale and bench-scale methods. The real-scale test environment was a post-flashover fire in a three-compartment (room, corridor, room) geometry, with the test specimens comprising wall lining materi-The bench-scale methods examined were the NBS cup furnace method and a new developmental protocol referred to as the 'SwRI/NIST' method. The N-gas Model was applied to the analysis of the data and was found to be consistent with most of the data. The methods were compared for similarity of gas yields, of primary gases, and of types of death. Differences were found in individual cases, but most of those were readily explainable on the basis of an understanding of the test conditions. As a result of these studies, a factor-of-3 agreement between bench-scale and real-scale results was established as both useful and practical.

PB91-178848 PC A03/MF A01 National Inst. of Standards and Technology (CAML), Gaithersburg, MD.

Gaithersburg, MD.

Boussinesq Algorithm for Enclosed Buoyant Convection in Two Dimensions.

R. G. Rehm, H. C. Tang, H. R. Baum, J. S. Sims, and D. M. Corley. Mar 91, 40p NISTIR-4540

Keywords: \*Convection, Computational fluid dynamics, Finite difference theory, Two-dimensional calculations, Stratified flow, Hydrodynamics, Algorithms, \*Building fires, \*Boussinesq flow.

Approximate equations for a Boussinesq model with viscous dissipation and thermal conduction describing buoyant convection driven by a heat source in a rectangular enclosure are derived. The finite difference algorithm for computing transient solutions in two dimensions to these equations is presented. The algorithm allows the enclosure fluid to be stratified in a direction parallel to the enclosure walls initially, or for gravity to have an arbitrary direction relative to the enclosure (but with no initial stratification). Computational results of transient, two-dimensional buoyant convection for very high resolution are presented. The hydrodyna-mics is directly based on the time-dependent Navier-Stokes equations; the model is valid in the Boussinesq approximation. No turbulence model or other empirical parameters are introduced. There is no inflow or outflow at boundaries; this assumption, although rather restrictive, allows the mathematical problem to be properly formulated so that no other empiricism is introduced by specification of the algorithmic boundary conditions. A finite-difference scheme second-order in space and first-order in time is used to integrate the evolution equations, and an elliptic solver is used to solve the pressure equation.

PB91-195222 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Center for Fire Research.

Engineering Analysis of Fire Development in the Hospice of Southern Michigan, December 15, 1985. Final rept.

H. E. Nelson. 1989, 12p Pub. in Proceedings of International Symposium on Fire Safety Science (2nd), Tokyo, Japan, June 13-17, 1988, p927-938 1989.

Keywords: \*Smoke, \*Fires, Investigations, Flashover, Fire safety, Combustion, Reprints.

An analysis of the development of fire and flow of smoke in a multi-fatality fire is presented. The analysis methods used are the least sophisticated available consistent with reasonable accuracy. Fire growth, flashover, pre- and post-flashover spread of products, and impact on victims are addressed. Issues relative to post-flashover combustion chemistry and post-flashover corridor flow are raised.

100,159 PB91-203620 PB91-203620 Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Fire Science and Engineering Div. Water Spray Suppression of Fully-Developed Wood Crib Fires In a Compartment.
Final rept.
J. Milke, D. Evans, and W. Hayes. 1985, 63p

See also PB88-232871. Sponsored by Federal Emergency Management Agency, Washington, DC. Pub. in Report of Test FR 3956, pt1 p1-63 Jan 85.

Keywords: \*Fire extinguishing agents, Water, Sprayers, Nozzle flow, Fire fighting, Fire tests, Experimentation, Reprints, Compartment fires.

A series of five experiments examining the effects of a simulated fire fighting water spray introduced into a fully-developed compartment fire were conducted for the Federal Emergency Management Agency by the Center for Fire Research at the National Bureau of Standards per Interagency Agreement (EMW-E-1239 Task Order 4A). Data from these tests were intended to be used as a check of predicted results from the Mission Research Corporation Fire Demand Model. The results illustrate the dynamics of compartment fire suppression using water sprays.

100,160 PB91-216820 PC A08/MF A02 National Inst. of Standards and Technology (BFRL), Gaithersburg, MD. **Building Technology Publications 1986-1989.** Final rept.

. A. Somers. Jun 91, 164p NISTIR-4616 See also PB88-110911.

Keywords: \*Buildings, \*Research management, \*Indexes(Documentation), \*Bibliographies, Laboratories, Civil engineering, Construction materials, US NIST.

The publication communicates the results of the Center for Building Technology's research during the period 1986 through 1989. Publications constitute a major end product to NIST's efforts. This publication is divided into six chapters: (1) alphabetical listing of publication titles, (2) keyword listing, (3) author listing, (4) title listings classified by NIST Publication Series and by non-NIST publishers such as a professional society. For the former, report titles are listed under six publicaror the former, report unless are listed unless six publica-tion designators: Building Science Series, Technical Notes, Special Publications, Journal of Research, Letter Reports, Interagency Reports, (5) technical dis-ciplines - Structures, Materials, Environment, and (6) report reference index used to identify report titles by using the report reference numbers from keywords in Chapter 2 and authors in Chapter 3.

100 161 PB91-217422 PC A05/MF A01 TriData Corp., Arlington, VA. Estimated Impact of the Center for Fire Research Program on the Costs of Fire.
P. Schaenman. Jun 91, 83p NIST/GCR-91/591 Sponsored by National Inst. of Standards and Technology (BFRL), Gaithersburg, MD.

Keywords: \*Fire safety, \*Cost analysis, Building codes, Economic analysis, Computerized simulation, Smoke detectors, Design standards, Safety engineering, Budgets, Fire detection systems, Flammability testing, CFR(Center for Fire Research).

The Center for Fire Research (CFR) has had a huge impact on reducing casualties and losses from fires. It also has helped stimulate new industries, and saved industry enormous sums by engineering fire safety better, averting business disruption, reducing liability, and in a number of other ways. The dividends of the past continue; CFR's budget essentially has been 'paid' through the Year 2100 by even the most conservative estimates of its impact. This was a first, brief effort to estimate the magnitude of the CFR impact, and how it is distributed across the major components of the total cost of fire. More work is needed on virtually every aspect of the estimation procedures used here. CFR's program has made a great contribution to life safety in the United States and has saved business billions of dollars in losses and unnecessary costs of fire. A much greater impact can be achieved with a few millions of dollars more investment in the CFR program each year - the enhanced program.

PB91-222604 PC A05/MF A01 National Inst. of Standards and Technology (BFRL),

Gaithersburg, MD. Reduction in Fire Hazard in Corridors and Areas Adjoining Corridors Provided by Sprinklers.

D. Madrzykowski. Jul 91, 90p NISTIR-4631
Sponsored by Public Buildings Service, Washington,

Keywords: \*Fire safety, \*Sprinklers, \*Corridors, Buildings, Graphs(Charts), Oxygen, Carbon dioxide, Carbon monoxide.

Full-scale fire tests were conducted in a noncombusti-ble burn room - corridor - target room test facility using wooden cribs as the fuel load. The facility was instrumented to measure gas temperatures and concentrations of oxygen, carbon dioxide and carbon monoxide. The combustion products were sampled at 1.5 m (5 ft) above the floor. The elevation is considered as a characteristic head height. Sprinklers were installed in the burn room and along the corridor. The sprinkler lines were instrumented with pressure switches and clocks to detect the activation time of the sprinklers. Depending on the test configuration, sprinklers were pressurized either with water for suppression ('wet') or air for measurement of activation time ('dry'). The sprinklers were allowed to activate automatically during the suppression tests.

100,163

PB91-231589 PC A03/MF A01 National Inst. of Standards and Technology (BFRL), Gaithersburg, MD.

General Routine for Analysis of Stack Effect.
J. H. Klote. Jul 91, 34p NISTIR-4588
Sponsored by General Services Administration, Washington, DC.

Keywords: \*Buildings, \*Fire tests, \*Air infiltration, Stacks, Computerized simulation, Smoke, Ventilation, Air flow

Stack effect is a major driving force of smoke movement in buildings. The paper presents a general method for evaluation of the location of the neutral plane for a space connected to its surroundings by any number of openings. A computer program, STACK, for analysis of the location of the neutral plane and result-ing flows is presented along with example analyses. The examples show that the location of the neutral plane between a space and its surroundings is a weak function of temperature and a strong function of the size of openings. Further, the mass flow rate leaving a space due to stack effect is a strong function of temperature.

100.164 PB91-240770 PC A03/MF A01 National Inst. of Standards and Technology (BFRL), Gaithersburg, MD.

Suppression of Post-Flashover Compartment Fires Using Manually Applied Water Sprays.
D. W. Stroup, and D. D. Evans. Jul 91, 41p NISTIR-

Sponsored by Swedish Fire Research Board, Stockholm, and Public Buildings Service, Washington, DC.

Keywords: \*Fire tests, \*Spraying, \*Water, Computerized simulation, Sprinkler systems, Buildings, Fla-

A series of four full scale fire tests were conducted to measure the effect of manual fire fighting efforts on post-flashover room fires. One objective of these tests was to generate data for evaluation of computer models of the fire suppression process. The tests were conducted in a room and corridor configuration consisting of a 2.44 m cube burn room connected to a 12.8 m long, 2.44 m wide, and 2.44 m high corridor. Hose nozzles with different water spray flow rates and medium drop sizes were used in each of the four nominally identical wood crib fires. Gas temperatures, wall surface temperatures and concentrations of oxygen, carbon dioxide, and carbon monoxide were measured in the burn room. Specialized aspirated and shielded thermocouples were used to minimize the effects of the water sprays on gas temperature measurements. The study showed that a water spray flowrate of 36.5 I find the study showed that a water spray howare of 35.3 filtrens with volume median drop size of 930 microns was just able to control the post-flashover fire, the flowrate of 16.3 1/min with median volume drop size of 800 microns did not control the fire, while the 79 1/min flowrate with volume median drop size of 1040 microns definitely extinguished the fire.

PB91-240788 PC A03/MF A01 National Inst. of Standards and Technology (BFRL),

Tramework for Utilizing Fire Property Tests.
T. G. Cleary, and J. G. Quintiere. Aug 91, 37p
NISTIR-4619

Keywords: \*Fires, \*Flammability testing, Buildings, Floors, Walls, Ceilings(Architecture), Flame propogation, Mathematical models.

#### General

A complete approximate set of equations is developed to describe fire spread and its resultant energy release over a surface. Wall, floor, and ceiling orientations are considered. The needed model data are couched in terms of available test method results, e.g., Cone Calorimeter and LIFT apparatuses. Several applications are presented to show how energy release rates can be predicted and how well they represent real data from full-scale and model room lining experiments.

100,166 PB92-109164 PC A16/MF A03 PB92-109164 PC A16/MF A03
National Inst. of Standards and Technology (NEL),
Gaithersburg, MD. Center for Fire Research.
Joint Panel Meeting of the UJNR Panel on Fire Research and Safety (11th). Held in Berkeley, CA. on
October 19-24, 1989.
N. H. Jason, and D. M. Cramer. Oct 90, 365p
NISTIR-4449
See also PB98 0315036

See also PB88-215926.

Keywords: \*Meetings, \*Fire safety, US NIST, Research management, Evacuating(Transportation), Carbon monoxide, Toxicity, Risk, Fire hazards, Safety engineering, Buildings.

The 11th Joint Meeting of the United States-Japan Panel on Fire Research and Safety was held on the campus of the University of California, Berkeley, October 19-24, 1989. Some disruption of the meeting resulted from the October 17 earthquake. The epicenter was about 60 miles southeast of San Francisco, in the Loma Prieta mountains near Santa Cruz. Thus, some Loma Prieta mountains near Santa Cruz. Thus, some of the papers were not presented, but are included in the volume. The volume comprises a total of 6 progress reports and 30 supporting papers in 3 areas: Risk, Hazard and Evacuation; Fire and Toxicity Chemistry; and Fire and Smoke Physics. The next Panel Meeting will be held in Japan in the autum of 1992.

100,167 PB92-110287

(Order as PB92-110261, PC A05/MF A01) National Inst. of Standards and Technology, Gaithersburg, MD.

Data for Room Fire Model Comparisons.

R. D. Peacock, S. Davis, and V. Babrauskas. c1991,

Included in Jnl. of Research of the National Institute of Standards and Technology, v96 n4 p411-462 Jul/Aug

Keywords: Data analysis, Fire tests, Buildings, Comparison, \*Building fires, \*Room fires, Fire models.

With the development of models to predict fire growth With the development of models to predict life growth and spread in buildings, there has been a concomitant evolution in the measurement and analysis of experimental data in real-scale fires. The report presents the type of analyses that can be used to examine large-scale room fire test data to prepare the data for comparison with zone-based fire models. Five sets of experimental data which can be used to test the limits of a typical two-zone fire model are detailed. A standard control of the proposition the growner of the set of nomenclature describing the geometry of the building and the quantities measured in each experiment is presented. Availability of ancillary data (such as smaller-scale test results) is included.

100,168 PB92-112218 PC A09/MF A03 National Inst. of Standards and Technology (BFRL), National list. of Standards and Technology (51712), Gaithersburg, MD. Summaries of BFRL Fire Research In-House Projects and Grants, 1991. N. H. Jason. Oct 91, 199p NISTIR-4686 See also PB91-216788 and report for 1989, PB90-

Keywords: \*Fire prevention, \*Fire tests, Research projects, Research management, Buildings, Combustion, Carbon monoxide, Smoke, Furniture, Evacuating(Transportation), Grants.

The report describes the research projects performed in the Building and Fire Research Laboratory (BFRL) Fire Research Program and under its grants program from October 1, 1990 through September 30, 1991. Contents: Carbon Monoxide Prediction; Soot Formation; Turbulent Combustion; Polymer Gasification; Toxic Potency; Furniture Flammability; Wall Fires; Fire Suppression: Fire Hazard Assessment: Engineering Suppression; Fire Hazard Assessment; Engineering Analysis Systems; Large Fires; Fire/Modeling Interactions; Fire Protection Technology.

100,169 PB92-112317

PC A04/MF A01

National Inst. of Standards and Technology, Gaithers-

burg, MD.
Engineering Analysis of the Fire Development in the Hillhaven Nursing Home Fire, October 5, 1989.
H. E. Nelson, and K. M. Tu. Sep 91, 57p NISTIR-

Sponsored by Health Care Financing Administration, Baltimore, MD.

Keywords: \*Fires, \*Nursing homes, Smoke, Fire tests, Flashover, Carbon monoxide.

The report presents the methods and results of an analysis of the development and spread of fire and smoke during the October 5, 1989 fire in the Hillhaven Rehabilitation and Convalescent Center, Norfolk, Virginia. The analysis uses data gathered from onsite visits, reports and information for other investigators, fire tests conducted at the National Institute of Stand-ards & Technology, and fire growth models and similar computations. The report details the procedure and data used, the reasons for those selected, and the results obtained. The analysis addresses mass burning rate; rate of heat release; smoke temperature; smoke layer depth; velocity, depth and temperature of the smoke front; oxygen concentration of smoke layer; carbon monoxide concentrations; and other factors. The areas of building analyzed include the room of fire origin, the corridor system exposed by that room, and other patient rooms on that corridor.

PC A05/MF A01 Pennsylvania State Univ., University Park. Dept. of Me-

chanical Engineering.

Turbulent Upward Flame Spread for Burning Verti-

Cal Walls Made of Finite Thickness.

Annual rept. 15 Aug 89-14 Aug 90.

A. K. Kulkarni, C. I. Kim, and C. H. Kuo. Sep 91, 88p. NIST/GCR-91/597

Grant NANB-8D0849 See also PB91-143297. Sponsored by National Inst. of Standards and Technology (BFRL), Gaithersburg, MD.

Keywords: \*Fire tests, \*Walls, Mathematical models, Buildings, Turbulent flow, Flame propagation, Mathematical models, Polyurethane, Wood, \*Upward flame spread.

The report presents the basic mechanisms of upward flame spread and develops a complete procedure to predict the flame spread on practical wall materials of finite thickness, appropriately verified by experiments. These objectives have been met. Specifically in the past year, several wall materials were tested in the upward flame spread apparatus, mathematical model development for predicting the upward flame spread was completed, and comparisons of data and predictions were made, in addition to completion of many other supporting tasks.

# **BUSINESS & ECONOMICS**

#### **Consumer Affairs**

100,171 PB92-112549 PC A03/MF A01 National Inst. of Standards and Technology (TS), Gaithersburg, MD. Weights and Measures Program.

Checking the Net Contents of Packaged Goods.

Third Edition, Supplement 2.

Final rept. C. S. Brickenkamp, and J. A. Koenig. Oct 91, 17p NIST/HB-133-ED-3-SUPPL 2 Also available from Supt. of Docs. as SN003-003-03111-9. See also PB91-107144.

Keywords: \*Packaging, \*Commodities, \*Labels, \*Handbooks, Requirements, Sampling, Revisions, Keywords: Tests, Procedures.

Only minor additions and revisions to NIST (formerly NBS) Handbook 133, Third Edition, 'Checking the Net Contents of Packaged Goods,' were adopted by the Conference in 1991. A few editorial changes have also

been made. The document consists of change pages to be added to Handbook 133, Third Edition, as amended by the 1990 Supplement.

#### Domestic Commerce, Marketing, & **Economics**

100,172

PB91-194415 PC A03/MF A01 National Inst. of Standards and Technology, Gaithersburg, MD. Office of Standards Services. Laboratory Accreditation in the United States.

M. A. Breitenberg. May 91, 31p NISTIR-4576 See also PB88-239793.

Keywords: \*Test facilities, \*Quality assurance, Calibration, Inspection, Tests, United States, USA, \*Laboratory accreditation, \*Accreditation.

The paper, the third in a series that includes NBSIR 87-3576, The ABC's of Standards-Related Activities in the United States, and NBSIR 88-3821, The ABC's of Certification Activities in the United States, is designed to provide information on laboratory accreditation to readers not entirely familiar with the topic. The report highlights some important aspects on the topic, furnishes information necessary to make informed decisions on the selection and use of laboratories, and serves as background for using other available documents and services. Readers interested in this area yalso wish to review NIST SP 808, Directory of Federal Government Laboratory Accreditation/Designary The paper, the third in a series that includes NBSIR 87-Federal Government Laboratory Accreditation/Designation Programs, which provides updated information on federal government laboratory accreditation and similar type programs conducted by the federal government. Companion volumes on state and local government and private sector laboratory accreditation programs are currently in preparation.

PB91-195693 Not available NTIS National Bureau of Standards, Gaithersburg, MD. Program Office.

Structural Change and Competitiveness: The U.S. Semiconductor Industry.

Final rept.

G. Tassey. 1990, 9p Pub. in Technological Forecasting and Social Change 37, n1 p85-93 Mar 90.

Keywords: Competition, Diversification, Strategy, Japan, USA, Reprints, \*Semiconductor industry, Competitiveness, Innovation.

Part of the difficulties being experienced by U.S. semiconductor firms in competing with the Japanese and several European firms can be explained by significant differences in industry structure. Specifically, semiconductors are produced by large electronics firms in Japan which have diversified into many downstream products, while U.S. firms still concentrate on semiproducts, while U.S. Irms still concentrate on semi-conductor components. The diversification smoothes the shocks of individual product cycles and increases the return on investment in semiconductor technology. Although some U.S. semiconductor firms have divers fied into several downstream product areas, the degree has not been sufficient and they have diversified hardly at all into related technologies with substantial economic potential such as optoelectronics.

PB92-108968 PC A05/MF A01 National Inst. of Standards and Technology, Gaithers-burg, MD. Office of Standards Code and Information. Directory of State and Local Government Labora-

Directory of State and Local Government Laboratory Accreditation/Designation Programs.
Special pub. (Final).
C. W. Hyer. Jul 91, 90p NIST/SP-815
Contract 43NANB017411
Also available from Supt. of Docs. as SN003-003-03093-7. Supersedes PB85-121390. See also PB91-167379 and PB91-194415. Sponsored by National Inst. of Standards and Technology, Gaithersburg, MD. Office of Standards Code and Information.

Keywords: \*Test facilities, \*Quality assurance, \*Directories, Calibration, Inspection, Tests, Laboratory accreditation.

#### Domestic Commerce, Marketing, & Economics

The directory is a guide to laboratory accreditation and similar types of programs conducted by state and local government agencies. These programs accredit or designate laboratories or other entities to conduct testing to assist the agencies in carrying out their responsibilities. The accreditation or designation is based on some type of assessment regarding the capability of the laboratory to conduct the testing. However, the nature of such assessments varies considerably from agency to agency. Entries in the directory are based primarily on information provided by each state and local government agency and reflect the agency's view of its activities.

PB92-126465 PC A03/MF A01 National Inst. of Standards and Technology, Gaithersburg, MD. Office of Standards Services.

Questions and Answers on Quality, the ISO 9000

Standard Series, Quality System Registration, and Related Issues.
M. Breitenberg. Nov 91, 24p NISTIR-4721
See also PB91-194415.

Keywords: \*Test facilities, \*International trade, \*Standards, \*Quality assurance, Assessments, Reliability, Inspection, Requirements, Engineering, Specifications, United States, European Community, \*Registrations, United States, tration, Laboratory accreditation, ISO 9000 Series.

The report provides information on the development, content, and application of the ISO 9000 standards to readers who are unfamiliar with these aspects of the standards. It attempts to answer some of the most commonly asked questions on quality; quality systems the content, application and revision of the ISO 9000 standards; quality system approval/registration; Euro-pean Community requirements for quality system approval/registration; and sources for additional help.

#### International Commerce, Marketing, & **Economics**

Not available NTIS National Bureau of Standards, Gaithersburg, MD. Office of Standards Code and Information. Domestic Implementation.

Final rept. 1983-85.

J. Overman. 1986, 18p Pub. in Report to the United States Congress on the Agreement on Technical Barriers to Trade - 'Stand-ards Code', Chapter V, p25-42 Feb 86.

Keywords: \*International trade, \*Standards, Barriers, United States, Exports, Industries, Regulations, Reprints, Trade Agreements Act.

The report describes the domestic implementation of the GATT Agreement on Technical Barriers to Trade (Standards Code) by the National Bureau of Standards (NBS) and the U.S. Department of Agriculture's Technical Office During the three pages and (1094) 1095 nical Office. During the three year period (1983-1985), NBS reported 59 proposed U.S. regulations to the GATT Secretariat; published 11 issues of tbt news; handled comments on 24 proposed foreign regula-tions; received 664 notifications of proposed regula-tions; answered over 6,000 requests for information; and provided standards-related technical assistance to manufacturers and exporters.

PB91-187823 PC A04/MF A01 National Inst. of Standards and Technology, Gaithersburg, MD. Office of Standards Code and Information. GATT Standards Code Activities of the National Institute of Standards and Technology 1990. Annual rept.

J. R. Overman. Apr 91, 53p NISTIR-4559 See also PB90-219817.

Keywords: \*International trade, \*Standards, Technical assistance, Certification, Regulations, Tables(Data), \*General Agreement on Tariffs and Trade, Notifications, Trade barriers, US NIST.

The report describes the GATT Standards Code activities conducted by the Standards Code and Information Program, National Institute of Standards and Technology (NIST), for calendar year 1990. NIST responsibilities include operating the U.S. GATT inquiry point for

information on standards and certification activities and the technical office for non-agricultural products; notifying the GATT Secretariat of proposed U.S. Federal Government standards-based rules that might sigorificantly affect trade; assisting U.S. industry with standards-related trade problems; and responding to inquiries about proposed foreign and U.S. regulations.

#### General

100,178
PB91-194498
Rational Inst. of Standards and Technology, Gaithers-National risk: of Standards and Technology, Gainlesburg, MD. Office of Standards Services.

Meeting of the Standards Working Group of the Joint U.S.-U.S.S.R. Commercial Commission (1st). Held in Moscow on March 11-13, 1991.

B. G. Simson. May 91, 235p NISTIR-4572

Keywords: \*Standardization, \*Meetings, International cooperation, Quality control, USSR, USA, Standards Working Group.

In a September 1990 Chairman's meeting of the Joint U.S.-U.S.S.R. Commercial Commission (JCC) in Moscow, senior officials from the U.S. Department of Commerce and the U.S.S.R. Ministry of Foreign Economic Relations established a Standards Working Group for the purpose of developing programs of mutual interest concerning standards development and conformity assessment. During its first meeting in Washington, D.C., and Gaithersburg, Maryland, on March 11-13, 1991, representatives from U.S. Governant, trade and otherspiral associations and standard standards. ment, trade and professional associations, and standard development associations provided the Soviet delegation with insights into U.S. standardization. The visitors described Soviet legislative initiatives now under development.

# CHEMISTRY

#### **Analytical Chemistry**

100,179 AD-A227 869/5 PC A02/MF A01 National Inst. of Standards and Technology, Gaithersburg, MD.

Scattered Light and Other Corrections In Absorption Coefficient Measurements in the Vacuum Ul-

traviolet: A Systems Approach.
R. Klein, W. Braun, A. Fahr, A. Mele, and H. Okabe.
Jun 90, 9p ARO-25911.2-CH,
Contract MIPR-119-89

Pub. in Jnl. of Research of the National Institute of Standards and Technology, v95 n3 p337-344 May-Jun

Keywords: \*Absorption coefficients, Automation, Auxiliary, Computers, Error analysis, Errors, Gases, Light scattering, Low intensity, Measurement, Reprints, \*Ultraviolet spectrometers, Systems approach, \*Vacuum ultraviolet radiation.

A systems approach in which computer automation is applied to a vacuum ultra-violet spectrometer and auxiliary components is described. The errors associated with the measurement of gaseous absorption coefficients in the vacuum ultraviolet are considered. The presence of scattered light introduces large errors particularly at those wavelengths where the source used is characterized by low intensity. In the case of a D2 light source this occurs in the region 120 to 130 nm. Simple considerations explain the variation of the absorption coefficient determinations in the presence of scattered light and lead to an appropriate treatment of the data to eliminate the error. Experimental results are presented illustrating the efficiency and precision obtainable with the present approach. Keywords: Absorption coefficient; Computer automation; Error analysis; Instrument; Vacuum; Reprints. (jhd)

100,180 AD-A243 170/8

PC A04/MF A01

National Bureau of Standards (NML), Gaithersburg, MD. Center for Chemical Physics

CID Spectra of Selected Target Molecules.

Final rep. Jul 84-Sep 87.

Final rep. Jul 84-Sep 87.

R. I. Martinez. Dec 89, 58p AFESC/ESL-TR-88-71,

Contracts MIPR-N84-56, MIPR-N84-56-A01

Supported in part by MIPR-N85-22, MIPR-N86-12,

MIPR-N87-12.

Keywords: Collisions, Cross sections, Data bases, Dissociation, Dynamics, Energy, Ions, Mass, Molecular properties, Molecules, Spectra, Standardization, properties, Molecules, Spectra, Standardization, Structures, Targets, Mass spectroscopy, \*Mass spectra, Quadrumpole moment, Identification, CID(Collisionally Induced Dissociation), Tandem mass spectrometers, Molecular dynamics.

This report describes research into the molecular dynamics of the collisionally induced dissociation (CID) process. This process occurs in tandem mass spectrometers, and is the major process by which primary or parent ions are converted into daughter ions of smaller mass. This work was undertaken in search of a means of standardizing conditions for tandem mass spectrometers so that standard spectral data bases could be collected and used to identify environmental unknowns. This research indicates that CID cross sections for the parent ions can be reproducibly measured as a function of collision energy, and are characteristic of the parent ion structures. Measurement of CID cross sections offers a new means of identifying unknown compounds.

PB91-147694 Not available NTIS National Bureau of Standards (NML), Gaithersburg,

MD. Chemical Kinetics Div.
Instrument-Independent Tandem Mass Spectrometry Database for XQQ Instruments: The Dynamical Prerequisites.

Final rept. R. I. Martinez. 1988, 6p Pub. in Rapid Commun. Mass Spectrom. 2, n1 p8-13 1988.

Keywords: \*Mass spectroscopy, \*Data bases, Computer aided design, Reprints.

The dynamical prerequisites are discussed in order to focus attention on design considerations for accomplishing an instrument independent MS/MS CAD Database for XQQ instruments.

100.182

Not available NTIS PB91-147769 National Inst. of Standards and Technology (NML), Caithersburg, MD. Organic Analytical Research Div.
Capillary Supercritical Fluid Chromatography of
Explosives: Investigations on the Interactions between the Analytes, the Mobile Phase and the Stationary Phase. Final rept.

A. Munder, S. Chesler, and S. Wise. 1990, 8p Pub. in Jnl. of Chromatography 521, p63-70 1990.

Keywords: \*Chromatographic analysis, \*Pressure, \*Temperature, \*Surface properties, Polarity, Siloxanes, Dipole moments, Explosives, Propellants, Solutes, Solid phases, Reprints, \*Supercritical fluid chromatography

The independent effects of pressure and temperature in supercritical fluid chromatography on the capacity ratio on chromatographic resolution of some polar organic model compounds were investigated. Increasing the pressure isothermally leads to a steady decrease in retention and resolution. With changing temperature, a maximum in the capacity ratio as well as the resolution was observed. These observations may be related to a combination of gas chromatographic (GC) and liquid chromatographic (LC) theories of solute interactions with the mobile and stationary phases. However, pure GC or LC-like behavior was not observed either below or above the critical point of the mobile phase. Capacity ratios for various explosives, propellants and related compounds were determined on capillary open tubular columns coated with either a non-polar methyl- or a polar cyanopropyl phenyl-sub-stituted siloxane stationary phase. The mobile phase for all studies was carbon dioxide. On the polar for all studies was calbul dioxide. On the polar column, many of the solutes exhibited a good correlation between their bulk dipole moment and chromatographic retention. Deviations from the correlation could be explained by means of the physical or steric properties of these solutes. The elution order of the

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## **Analytical Chemistry**

compounds on the non-polar column was similar to the order achieved using GC rather than LC.

100, 183 PB91-147777 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Gas and Particulate Science Div. Use of Single Particle Standards for LAMMA Call-

Final rept.
I. H. Musselman, D. S. Simons, J. A. Small, and R. W. Linton. 1986, 17p

Pub. in Jnl. of Trace and Microprobe Techniques 4, n3 p197-213 1986.

Keywords: \*Microanalysis, \*Standards, Isotope ratio, Calibration, Reprints, \*Laser microprobe mass spectroscopy.

Single particle standards are being used in the development and testing of the relatively new technique of laser microprobe mass analysis (LAMMA). Experiments being conducted at the National Bureau of Standards include the use of particle standards to cali-brate isotopic measurements, to investigate detection limits and the accuracy of isotopic analysis in submicrometer particles, and to determine the feasibility of nickel speciation by LAMMA.

100,184 PB91-148148 Not available NTIS
National Bureau of Standards (NML), Gaithersburg,
MD. Organic Analytical Research Div.
Trace Determination of Critic Research Line Preconcentration. Final rept.

A. Syty, R. G. Christensen, and T. C. Rains. 1986, 4p. Pub. in Atomic Spectroscopy 7, n4 p89-92 1986.

Keywords: \*Chromium, \*Chromates, \*Liquid chromatography, \*Atomic spectroscopy, Concentrating, Spectrochemical analysis, Surface waters.

A liquid chromatography/atomic absorption spectro-A liquid chromatography atomic absorption spectro-metric (LC/AAS) technique for the direct determina-tion of Cr(VI) at ng/mL in the presence of Cr(III) is de-scribed. In this method Cr(VI) is preconcentrated on a C-18 bonded silica column. The column is connected directly to the aspirating capillary of an atomic absorp-tion spectrometer (AAS). After a preconcentration step the Cr(VI) is eluted from the column directly into the AAS unit where the chromium absorbance is measured. A preconcentration factor of 300 is attained using a 25-cm long column. The method has been evaluated using samples of natural pond water with 100 percent recovery of spiked Cr(VI).

100,185 PB91-148502 PC A06/MF A01 National Inst. of Standards and Technology (NML), Boulder, CO. Thermophysics Div. Strategy for Chemical Analysis of Alternative Refrigerants.

Technical note. J. Bruno. Aug 90, 102p NIST/TN-1340 Also available from Supt. of Docs.

Keywords: \*Refrigerants, \*Substitutes, \*Mass spectroscopy, \*Gas chromatography, \*Infrared spectroscopy, Fluorohydrocarbons, Purity, Contaminants, Water analysis, Adsorbents, Volummetric analysis, Hy-

The chemical purity of samples of alternative refrigerants which are used in the determination of the thermophysical properties is of paramount importance. Many properties, such as vapor-liquid equilibria and transport properties such as thermal conductivity, require that measurements be performed on as pure a awaterial as possible. Some common impurities such as water can have an extremely deleterious effect on a measurement, while the effects of other impurities are more subtle. Alternative refrigerants which are not available at purity levels that are normally considered 'research grade' must be characterized in order for the data to be properly interpreted, and for the reported results to be used appropriately. In addition, it is necessary to assess the reactivity of alternative refrigerants in the presence of many of the common construction materials used in experimental apparatus. The National Institute of Standards and Technology has evolved an analytical protocol which is applied to each system. In the paper, the various analytical methods will be dis-cussed, and the data of general usefulness presented. In addition, some of the novel instrumental approaches employed at NIST will be described.

100, 186 PB91-148817 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Inorganic Analytical Research Div. Characterization of the Mineral Fraction in Botani-cal Reference Materials and Its Influence on Homogeneity and Analytical Results.

R. M. Lindstrom, A. R. Byrne, D. A. Becker, B. Smodis, and K. M. Garrity. 1990, 3p Pub. in Fresenius Jnl. of Analytical Chemistry 338, p569-571 1990.

Keywords: \*Trace elements, \*Leaves(Botany), \*Standards, \*Inorganic materials, Neutron activation analysis, Microscopy, Heterogeneity, Cyclone separators, Reprints, Standard reference materials.

The NIST natural-product leaf Standard Reference Materials have been widely used in developing reliable methods of analysis. A small amount of mineral matter present in these materials was separated by flotation, and characterized qualitatively by microscopy and quantiatively by neutron activation analysis. Several elements are concentrated in the mineral fraction, which can lead to analytical error through incomplete dissolution or sampling statistics. Two new candidate materials prepared by the Office of Standard Reference Materials, SRM 1515 Apple Leaves and SRM 1547 Peach Leaves, have been processed with an airjet mill, resulting in a very finely ground leaf material, with particle size less than 200 mesh. A cyclone classifier in the process discriminates against coarse grit, so that the content of minerals in the ground material is less than in the first-generation materials. Better homogeneity was in fact observed, even down to 100 mg sample size. One must use caution, however, to assure that any inhomogeneity found in real samples are appropriately considered and dealt with.

100,187 PB91-148858 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Organic Analytical Research Div.
Reverse-Phase HPLC Separation and Electrochemical Detection of Retinol and Its Isomers.

W. A. MacCrehan, and E. Schonberger. 1987, 14p Pub. in Jnl. of Chromatography - Biomedical Applica-tions 417, n1 p65-78 1987.

Keywords: \*Retinol, \*Liquid chromatography, \*Vitamin A, Isomers, Blood serum, Electrochemistry, Ultraviolet detectors, Reprints.

Baseline separation of all of the isomers of retinol using reverse-phase liquid chromatography in under 30 minutes is presented. A new approach to the detection of retinol using electrochemical detection is developed. The oxidative electrochemistry of retinol is studied using coulometry and HPLC. The new approach is compared to UV/visible absorbance detection for the determination of retinol in human serum extracts.

100.188 PB91-148874 Not available NTIS
National Bureau of Standards (NML), Gaithersburg,
MD. Inorganic Analytical Research Div.
Research at NBS in Direct Potentiometric Meas-

urements in Blood. Final rept

G. Marinenko, P. C. Gunaratna, and W. F. Koch.

Pub. in Proceedings of Meeting of the European Working Group on Ion-Selective Electrodes (8th), Graz, Austria, October 2-4, 1986, p269-279 1987.

Keywords: \*Calcium ions, \*Potassium ions, \*Sodium ions, \*Blood, \*Activity coefficients, \*Potentiometric analysis, Electrolytes, Ion selective electrodes, Electrochemical cells, Mercury amalgams, Reprints.

A research project, sponsored by the National Committee for Clinical Laboratory Standards and funded by several manufacturers' of clinical potentiometric instruments, has been initiated in the Electroanalytical Research Group at the National Bureau of Standards. The goal of the research is to develop reference methods and materials for measuring the activity of free ionized sodium, potassium, and calcium in blood by direct potentiometry with ion selective electrodes. The initial thrust of the research will focus on sodium, wherein it is anticipated that the definitive method for the sodium activity measurements will be the sodium analgam cell. A synopsis of the program and the theory supporting

the approach will be given. In preparatory work leading to the use of the analgam cell, a new cell with low liquid junction potential has been constructed for use with ion selective electrodes. Dilute ammonium chloride is used as the reference filling solution and agar bridge electrolyte. Preliminary results using the cell for comparing activity and concentration measurements will be discussed. The relative accuracy of the measured activity of sodium using a variety of free sodium ion probes has been evaluated. The sodium analgam cell has been designed and constructed. Preliminary testing of the cell is now underway and appears very prom-

100,189

Not available NTIS PR91-148981 National Bureau of Standards (IMSE), Gaithersburg, MD. Polymers Div.

Methods for the Analysis of Organometallic Compounds in Wastes.

Final rept. G. J. Olson, F. E. Brinckman, and W. R. Blair. 1988,

16<sub>D</sub> Sponsored by Office of Naval Research, Arlington, VA.

Pub. in Waste Testing and Quality Assurance, ASTM STP 999, p130-145 1988.

Keywords: \*Organometallic compounds, \*Chemical analysis, \*Environmental surveys, Toxic hazards, Waste disposal, Water pollution sampling, Chromatography, Separation processes, Trace elements, Reprints, Chemical specification.

Organometallic compounds occur in the environment as a result of anthropogenic and biogenic processes. Since rganiometals are often much more toxic than the corresponding inorganic forms of metals, it is important to be able to speciate the forms of metals in envi-ronmental samples at ultratrace levels. Chemical speciation methods, based on the use of chromatographic separations followed by element-selective detection, have been developed in the laboratories and elsewhere. These methods, described in part in the paper, are helping the analysis of organometal species at their action levels (down to parts-per-trillion levels) in environmental matrices, leading to a better under-standing of environmental occurrence, fate, effects, and transformation. New methods for nondestructive analysis of metal species on surfaces are under development.

100.190

PB91-149187 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Organic Analytical Research Div. Determination of Bonded Phase Thickness in Liquid Chromatography by Small Angle Neutron Scattering. Final rept.

L. C. Sander, C. J. Glinka, and S. A. Wise. 1990, 3p Pub. in Analytical Chemistry 62, n10 p1099-1101 1990.

Keywords: \*Bonded coatings, \*Silicon dioxide, \*Thickness, Porosity, Adsorbents, Liquid chromatography, Neutron scattering, Surface properties, Alkylation, Penetration, Methanol, Reprints.

Preliminary results of research using the technique of small angle neutron scattering (SANS) to characterize phase morphology of alkyl modified silica is reported. phase morphology of alkyl modified silica is reported. The technique of contrast variation was used to reduce scattering interferences from the pore structure. With this procedure, the scattering experiments are carried out on the sample in a liquid environment. By varying the deuterium/hydrogen ratio of the liquid (e.g., D2O/H2O ratio), the scattering length density (sld, essentially the index of refraction for neutrons) of the liquid can be varied. This permits the pore structure to be masked by matching the sld of the silica. The thickness of the bonded phase layer was determined for various alkyl modified substrates. In addition, the for various alkyl modified substrates. In addition, the degree of solvent penetration (volume fraction of methanol associated with the alkyl chains) was determined. The significance of bonded phase thickness to column properties is briefly discussed.

100.191

Not available NTIS PB91-158865 National Inst. of Standards and Technology (NML), Gaithersburg, MD. Inorganic Analytical Research Div.

# **Analytical Chemistry**

NIST Standards for Sodium and Potassium.

W. F. Koch. 1990, 9p Pub. in Proceedings of International Symposium on Metrology and Clinical Applications of Electrochemical and Fiber Optic Sensors, Rochester, MN., September 22-25, 1989, p3-11 1990.

Keywords: \*Potassium, \*Sodium, \*Blood serum, \*Standards, Ion selective electrode analysis, Laboratory tests, Precision, Chemical analysis, Reprints.

The collaborative research project with manufacturers and users of clinical potentiometric instruments, sponsored by the NCCLS and conducted at the National Institute of Standards and Technology (NIST), is nearing attainment of its primary goal to bring conformity to the direct potentiometric measurements of sodium and potassium in human serum through the development of reference materials. Based on the results of the fourth interlaboratory test a candidate Standard Reference Material (SRM) has been produced by the Technicon Corporation, according to the specifications of the steering committee of the NCCLS project. The material was prepared from a single human serum pool, processed, ultra-filtered, and spiked with sodium and potassium resulting in three levels, nominally 120, 140, and 160 mmol/L sodium, and correspondingly, 6, 4, and 2 mmol/L potassium. All other components in the and 2 minor/L potassion. All other components in the sera are at normal levels. The three sera were dispensed into 4-mL glass ampules (3.2 mL per ampoule) and frozen at -50 C. The material is designated as SRM 956, Electrolytes in Human Serum. To test the efficiency of the material, a fifth interlaboratory test was conducted among eight manufacturers and three hospitals, using the candidate SRM and the prototype material from the fourth test. The results of the test indicate a significant improvement in interlaboratory precision when data are subjected to post-calibration. SRM 956 is now in the final stages of certification for sodium and potassium total concentration. These two analytes have been analyzed by the definitive methods (gravimetry and isotope dilution mass spectrometry, respectively) at NIST and the reference flame methods at NIST and two other cooperating laboratories.

100,192 PB91-162198 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Inorganic Analytical Research Div. Low-Background Gamma-Ray Assay Laboratory for Activation Analysis.

Final rept. R. M. Lindstrom, D. J. Lindstrom, L. A. Slaback, and

J. K. Langland. 1990, 5p Pub. in Nuclear Instruments and Methods in Physics Research A299, p425-429 1990.

Keywords: \*Activation analysis, \*Gamma counters, Background radiation, Radiation shielding, Cosmic neutrons, Cosmic rays, Comparison, Reprints.

The sources of background in a gamma-ray detector were experimentally determined in underground and surface counting rooms, and an optimized shield was constructed at NIST. The optimum thickness of lead was 10-15 cm, with a greater thickness giving an increased background due to the buildup of tertiary cosmic-ray particles. Neither cadmium, tin, copper nor plastic (hydrocarbon or fluorocarbon) was desirable as a shield liner, since all these increased the background continuum or introduced characteristic peaks into the background spectrum. Two broad peaks in the background result from inelastic scattering of cosmic-ray neutrons (0.02/sq cm/s) in germanium. These neu-trons also excite the lower nuclear levels of lead and structural iron to produce additional gamma-ray peaks in the spectrum. The influence of the 20 MW NIST rein the spectrum. The influence of the 20 MW NIST reactor, located 60 m from the detector, was undetectable. Comparisons among detectors and locations clearly separate cosmic from environmental components of the background.

100, 193 PB91-162297 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Electron and Optical Physics Div. Resonance Ionization Spectroscopy/Resonance Ionization Mass Spectrometry Data Service. II. Data Sheets for AI, Ca, Cs, Cr, Co, Cu, Kr, Mg, Hg, and Ni

Final rept. E. B. Saloman. 1991, 60p Pub. in Spectrochimica Acta 46B, n3 p319-378 1991.

Keywords: \*Resonance ionization mass spectroscopy, \*Chemical analysis, Aluminum, Calcium, Cesium,

Chromium, Cobalt, Copper, Krypton, Magnesium, Mercury, Nickel, Reprints, \*Resonance ionization spec-

A data service has been established at the National Institute of Standards and Technology to provide the necessary information to apply the techniques of Resonance Ionization Spectroscopy (RIS) and Resonance Ionization Mass Spectrometry (RIMS) to routine use in analytical chemistry. The service collects and calculates the relevant atomic data, chooses appropriate resonance ionization schemes, and indicates pertinent operating details of successful RIMS studies. The first operating details of successful RIMS studies. The first group of data sheets was published previously covering the elements As, B, Cd, C, Ge, Au, Fe, Pb. Si and Zn. The second group of data sheets is presented here. It covers the elements Al, Ca, Cs, Cr, Co, Cu, Kr, Mg, Hg and Ni. Others will be published periodically. Reprints of RIS/RIMS work are solicited so that those efforts may be included in future data sheets.

100,194 PB91-174235 Not available NTIS National Inst. of Standards and Technology, Gaithersburg, MD. Standard Reference Materials Program. Appendix: Standard Solutions and Certified Reference Materials.

Final rept.

R. Alvarez. 1990, 9p Pub. in Official Methods of Analysis, v2 p1214-1222

Keywords: \*Standards, \*Solutions, Chemical analysis, Data, Reprints, \*Certified reference materials, \*Standard reference materials.

The appendix gives the methods to make standard solutions and some standard reference materials.

100.195

PB91-187641

(Order as PB91-187617, PC A06/MF A01) National Inst. of Standards and Technology, Gaithersburg, MD.

Multiple Variable-Angle Light Scattering Detector

for Gel Permeation Chromatography.

P. H. Verdier. 1991, 13p Included in Jnl. of Research of the National Institute of Standards and Technology, v96 n2 p177-189 Mar/Apr

Keywords: \*Gel permeation chromatography, \*Light scattering, \*Molecular weight, Optical detectors, Polystyrene, Polymers.

A light scattering detector has been designed and constructed for use with gel permeation chromatographs. The detector measures light scattered from the eluting sample simultaneously at nine scattering angles, and is connected to a computer-controlled display which exhibits the angular dependence of the scattering in real time while the sample is eluting. Use of the lightscattering detector in conjunction with the usual con-centration-sensitive detector allows the direct determination of molecular weight as a function of elution volume, thereby making the chromatographic system 'self-calibrating.' Tests of the system with a series of linear and branched polystyrenes suggest that it will be a useful tool for the study and characterization of branched polymers.

100,196 PB91-189282 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Inorganic Analytical Research Div. Second Dissociation Constant and pH of N-2-hydroxyethylpiperazine-N'-2-ethanesulfonic Acid (HEPES) from 0 to 50C.

Final rept. D. Feng, Y. C. Wu, and W. F. Koch. 1989, 6p Pub. in Analytical Chemistry 61, n13 p1400-1405 1989.

Keywords: \*HEPES, \*Buffers(Chemistry), \*pH, \*Chemical equilibrium, \*Dissociation, Sodium chloride, Thermodynamic properties, Electrical potential, Re-

HEPES (N-2-Hydroxyethylpiperazine-N'-2-ethanesul-fonic acid) has been recommended as a pH buffer for physiological measurements. The pH values for thre buffer system at ionic strengths similar to those in physiological fluids have been determined at temperatures from 0 to 50 C by the emf method. The influence of NaCl on the buffer and the liqued junction potential associated with the salt have been evaluated. Thus, the practical, operation pH value can be ascertained.

The second dissociation constant of HEPES has been determined and the thermodynamic properties have been calculated.

100,197

PB91-189860 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Electricity Div.

Detection of Trace Disulfur Decafluoride in Sulfur Hexafluoride by Gas Chromatography/Mass Spectrometry.

Final rept.

J. K. Olthoff, R. J. Van Brunt, J. T. Heron, and I. Sauers. 1991, 7p Sponsored by Department of Energy, Washington, DC.

Office of Electrical Systems.

Pub. in Analytical Chemistry 63, n7 p726-732, 1 Apr 91.

Keywords: \*Sulfur fluorides, \*Sulfur hexafluoride, \*Mass spectroscopy, \*Gas chromatography, Chemical analysis, Pyrolysis, Hydrolysis, Reprints.

A new method is described for detection of S2F10 in SF6 in the parts-per-billion (ppb) level. The method utilizes a gas chromatograph/mass spectrometer (GC/ IIZES a gas chromatograph/mass spectrometer (GC/MS) equipped with a heated jet separator. S2F10 is converted to SOF2 on the hot surfaces of the low-pressure portions of the jet separator at temperatures above 150 C by a surface-catalyzed reaction involving H2O. As a consequence of the conversion, peaks corresponding to S2F10 appear on single-ion chromatograms at ion masses characteristic of SOF2 (m/z=48, 67, and 86) where there is little or not interference from features. But this method, a direct peakels of SE6 for features. By this method, a direct analysis of SF6 for S2F10 content can be performed with greater sensitivity than conventional gas chromatographic methods and with a higher degree of reliability and in a time much shorter than required for chromatographic methods that use enrichment procedures. Problems associated with the preparation and stability of reliable S2F10 reference samples are discussed.

100,198

PB91-189878 PB91-189878 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Inorganic Analytical Research Div. Introduction to Supercritical Fluid Chromatography. 1. Principles and Instrumentation.
Final rept.

M. D. Palmieri. 1988, 1p See also Part 2, PB89-230312.

Pub. in Jnl. of Chemical Education 65, n10 pA254 1988

Keywords: \*Supercritical fluid chromatography, Laboratory equipment, Gas chromatography, Liquid chromatography, Reviews, Reprints, \*Supercritical fluids.

The basic characteristics of supercritical fluids are described. Supercritical fluids are used as mobile phases in chromatography, and various aspects of supercritical fluid chromatography (SFC), liquid chromatography, and gas chromatography are compared. Finally the basic instrumentation required to perform SFC is described.

100, 199

PB91-190041 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Organic Analytical Research Div.

Evaluation of Column Performance in Liquid Chromatography.

Final rept.

L. C. Sander, 1988, 8p Pub. in Jnl. of Chromatographic Science 26, n8 p380-387 1988.

\*Liquid chromatography, Keywords: Absorbers(Equipment), Surface properties, Reviews, Selectivity, Performance evaluation, Reprints, Silanol activity, Trace metal activity.

Procedures for the evaluation of chromatographic properties of LC columns are described in the review. General tests for assessing silanol activity, hydropho-bicity, trace metal activity, phase type (monomeric vs. polymeric chemistry), and pore size are presented. Also included are specific tests for various solute classes. An emphasis is placed on practical aspects of column testing, and characterization procedures that require bulk packing material (i.e., unpacking the column) have been largely excluded.

#### CHEMISTRY

### **Analytical Chemistry**

100,200 PB91-195156 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Inorganic Analytical Research Div.
High Purity Chemicals and Clean Rooms for Trace

Metal Analysis.

Final rept.

Pub. in Proceedings of International Symposium on Trace Analysis in Environmental Samples and Standard Reference Materials, Honolulu, Hl., January 6-8, 1988, p97-100.

Keywords: \*Trace amounts, \*Metals, \*Chemical laboratories, Purity, Clean rooms, Reprints, \*Trace analysis, \*National Bureau of Standards, Environmental samples, Analytical blanks.

The experience of the analytical laboratories at NBS in performing trace metal analysis in environmental samples is analyzed. Specifically, the role of ultra-pure reagents and clean laboratories in reducing the analytical blank is related to significant requirements for environmental samples.

100,201 PB91-195164 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Inorganic Analytical Research Div.

Recommended Inorganic Chemicals for Calibration.

Final rept. J. R. Moody, K. W. Pratt, T. C. Rains, and R. R. Greenberg. 1988, 1p Pub. in Analytical Chemistry 60, n21 p1203 1988.

Keywords: Primary standards, Chemical compounds, Stoichiometry, Purity, Calibration, Chemical analysis, Reprints, \*Standard solutions.

Compounds and metals have been critically reviewed in terms of their suitability for use in preparing primary standard solutions for instrumental calibrations. Methods for preparing solutions from these chemicals are discussed. The tables list the available forms and purities for all but the radioactive elements and rare earth gases. A discussion of the relevance of purity, stoichiometry, and assay of chemicals for the analyst is given.

100,202 PB91-195180 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Gas and Particulate Science Div. Strategies for Background Subtraction in Electron Probe Microanalysis X-ray Compositional Mapping. Final rept.

R. L. Myklebust, D. E. Newbury, and R. B.

Marinenko. 1989, 7p Pub. in Analytical Chemistry 61, n15 p1612-1618 1989.

Keywords: \*Electron probes, \*X-ray analysis, \*X-ray spectroscopy, \*Spectrum analysis, \*Background discrimination, Ouantitative analysis, Atomic properties, Reprints, \*Compositional mapping.

The background subtraction methods necessary for quantitative compositional mapping with an electron microprobe is discussed. Compositional maps are pre-sented which demonstrate the need for determining a background dependent on average atomic number of the area of the specimen being analyzed. The measurement techniques and requirements for WDS, EDS and combined EDS/WDS compositional maps are dis-cussed. The corrections for EDS analyses are built into the measurement method while for WDS analyses, the average atomic number of each analyzed point must be determined in order to compute the background at that point.

100.203 PB91-195479 Not available NTIS National Inst. of Standards and Technology (CSTL), Gaithersburg, MD. Surface and Microanalysis Science

Inner-Shell Ionization Cross Sections. Final rept.

C. J. Powell. 1990, 8p

Pub. in Microbeam Analysis - 1990, p13-20.

Keywords: \*Inner-shell ionization, \*Ionization cross sections, \*Microanalysis, Auger electron spectroscopy, X ray analysis, Electron impact, Reprints, Electron probe microanalysis, Electron energy loss spectrosco-

Values of cross sections for ionization of inner-shell electrons by electron impact are required for electron probe microanalysis, Auger-electron spectroscopy, and electron energy-loss spectroscopy. The present author has previously reviewed measurements and calculations of inner-shell ionization cross sections, and the present paper is an update and summary of the earlier reviews with emphasis on data for total inner-shell ionization cross sections as needed for x-ray microanalysis. Information is given on the more useful formulae for ionization cross sections and the extent to which they agree with calculations and measurements for particular elements.

100,204 PB91-195727 PB91-195727 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Gas and Particulate Science Div. Accuracy of Transmission Electron Microscopy Analysis of Asbestos on Filters: Interlaboratory Study. Final rept

S. Turner, and E. Steel. 1991, 5p See also PB87-162111.

Pub. in Analytical Chemistry 63, n9 p868-872, 1 May

Keywords: \*Asbestos, \*Electron microscopy, \*Accuracy, \*Fibers, Laboratory tests, Filters, Statistical analysis, Interlaboratory comparisons, Reprints.

An interlaboratory study was conducted to determine the accuracy of determinations of the asbestos con-centration on filters by use of transmission electron microscopy. Replica sections were prepared from a single polycarbonate filter that had chrysotile and several types of non-asbestos particles deposited on its surface. Twenty-seven analysts from 15 laboratories counted a minimum of 3 grid squares and recorded the physical characteristics of the particles and the methods used for identification of the particles. One of the grid squares counted by each analyst was reanalyzed at the National Institute of Standards and Technology (NIST) by using verified counting methods. The mean value of TP/TNS (true positives/total number of structures) obtained by the laboratories on the verified grid squares is 0.67, and the mean value for FP/TNS (false positives/total number of structures) is 0.04. More than 40% of the fibers shorter than 1 micrometer were missed, whereas less than 20% of the fibers longer than 1 micrometer were missed by the analysts. Incor-rect translation of the electron microscope stage is a likely cause of many false negative values. Other possible reasons for false negatives and false positives are discussed.

100,205 PB91-203893 Not available NTIS National Inst. of Standards and Technology, Gaithersburg, MD. Office of Measurement Services Reference Materials for Analytical Chemistry.

S. D. Rasberry. 1991, 3p Pub. in Analusis 19, n1 p3**5**-37 Jan 91.

Keywords: \*Standards, \*Chemical analysis, Accuracy, Reprints.

With every passing year, the role of analytical chemistry seems to increase in prominence. This may be so for several reasons, but perhaps most importantly because good measurement is a key to higher productivity. Industrialists are eager to improve quality assur-ance while reducing wasted energy, manufacturing re-jects, and product liability problems. Patients in hospitals are eager to have accurate clinical analyses to support proper diagnoses and treatment. All mankind is eager for more accurate environmental analyses to help protect the long-term future of our planet.

PB91-203901 Not available NTIS National Inst. of Standards and Technology, Gaithersburg, MD. Office of Measurement Services Role of Reference Materials in Quality Assurance. Final rept.

S. D. Rasberry. 1990, 2p

Pub. in Analytical Proceedings 27, n11 p296-297 Nov

Keywords: \*Chemical analysis, \*Ouality assurance, Standards, Decision making, Measurement, Reprints, \*Reference materials, National Institute of Standards and Technology

Analytical measurements are increasingly important to industrial quality assurance (OA) and to critical decision making in such fields as clinical, nutritional, and environmental chemistry. Several factors important to attaining analyses that are reliably accurate will be noted. The summary will focus on the role of reference materials in accurate chemical analysis. Fundamental attributes of reference materials will be described, together with details on how they serve as benchmarks for the measurement process. Some examples will be drawn from materials recently certified at the National Institute of Standards and Technology (NIST).

100,207

PB91-203968 Not available NTIS
National Inst. of Standards and Technology (NML),
Gaithersburg, MD. Radiation Physics Div.
Resonance Ionization Spectroscopy/Resonance
Ionization Mass Spectrometry Data Service.
Final rept

Final rept. E. B. Saloman. 1989, 4p

See also PB91-162297.

Pub. in Proceedings of the International Symposium on Resonance Ionization Spectroscopy and Its Applica-tions (4th), Gaithersburg, MD., April 10-15, 1989, p255-

Keywords: \*Mass spectroscopy, \*Chemical analysis, \*Information systems, Cross sections, Data, Oscillator strength, Reprints, \*Resonance ionization spectroscopy, \*Resonance ionization mass spectrometry.

A data service is being established at the National Bureau of Standards to provide the necessary information to apply the technique of Resonance lonization Mass Spectrometry (RIMS) to routine use in analytical chemistry. This service will collect and calculate the relevant atomic data, choose appropriate resonance ionization schemes, and indicate pertinent operating details of successful RIMS studies. A sample data sheet is included and others will be available at the Symposium. Suggestions are solicited on how to improve the format and content of the data sheets.

PB91-236596 Not available NTIS National Inst. of Standards and Technology (CSTL), Gaithersburg, MD. Surface and Microanalysis Science

Quantitative Analysis of Impurities in SIMOX Samples Using Secondary Ion Mass Spectrometry.
Final rept.

P. H. Chi, D. S. Simons, and P. Roitman. 1991, 5p Pub. in Surface and Interface Analysis 17, p57-61 1991.

Keywords: \*Gas-solid interfaces, \*Silicon, \*Ion implantation, \*Ouantitative analysis, \*Annealing, Mass spectroscopy, Ion microprobe analysis, Microanalysis, Impurities, Process variables, Surface chemistry, Temperature dependence, Time dependence, Chemical analysis, High temperature tests, Diffusion, Nitrogen, Aron Oversion, Seprints, Simon process Argon, Oxygen ions, Reprints, Simox process.

Silicon films produced by the SIMOX process (separation by implanted oxygen) must be annealed at high temperature to remove the crystal damage introduced during implantation of the high oxygen dose. Different annealing gases, temperatures and times have been investigated. In such processes, various impurities present in the high-temperature ceramic furnace tube, as well as annealing gas species, may be incorporated into the samples. Secondary ion mass spectrometry (SIMS) is used as a quantitative tool to analyze the diffusion of tube components and gases into annealed SIMOX samples. Samples prepared for the investigation were annealed in nitrogen and argon at temperatures ranging from 1250 to 1350 C. It was found that most impuritites are present at low levels and are generally trapped in the surface oxide that is grown during the anneal. SIMS analyses of SIMOX samples an-nealed in nitrogen showed that nitrogen tends to col-lect in both the surface oxide and buried oxide layers, piling up at the oxide/silicon interfaces.

100,209

PB91-237727 Not available NTIS National Inst. of Standards and Technology (CSTL), Gaithersburg, MD. Inorganic Analytical Research Div. Characteristics of Aerosols Produced by the Spark Discharge.

Final rept. R. L. Watters, J. A. Small, F. H. Shen, J. R. DeVoe, and R. B. Marinenko. 1989, 8p Pub. in Analytical Chemistry 61, n17 p1826-1833 1989.

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# **Analytical Chemistry**

Keywords: \*Electric discharges, \*Metals, \*Aerosols, Brasses, Copper zinc alloys, Chemical analysis, Spectroscopy, Electron microscopy, Chemical composition, Physical properties, Reprints, Spark erosion craters.

A detailed study of the physical properties and the chemical composition of spark-produced aerosol and corresponding erosion craters has been undertaken. A high repetition rate (1 kHz), electronically controlled waveform spark source was used to generate the aerosol from samples of standard reference materials. The feasibility of using an on-line electrical mobility an-alyzer to monitor real-time particle concentrations was examined. Consistent bias in the Zn/Cu ratios of aerosols from a series of brass SRMs corresponded to a reverse bias in the Zn/Cu ratios measured in the spark erosion pits. Collected particles were dissolved and analyzed by inductively coupled plasma spectrometry. A predominance of small particles (100 A) was observed and confirming analyses using the analytical electron microscope was used on individual particles.

PB92-116755 PB92-116755 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Inorganic Analytical Research Div.

Laser Enhanced Ionization as a Selective Detector for Liquid Chromatographic Determination of Alkyltins in Sediment.

Final rept. K. S. Epler, T. C. O'Haver, W. A. MacCrehan, and G. C. Turk. 1988, 5p Sponsored by Maryland Univ., College Park. Dept. of

Chemistry and Biochemistry.
Pub. in Analytical Chemistry 60, n19 p2062-2066 1988.

Keywords: \*Tin organic compounds, \*Detectors, \*Liquid chromatography, \*Sediments, Reprints, \*Liquid chromatography, \*Sediment: \*Laser enhanced ionization, \*Trialkyltins.

Laser-enhanced ionization (LEI), used as an elementspecific detector for liquid chromatography (LC), is applied to trialkyltin determinations in sediment. The high sensitivity of LEI compensates for the degradation in detection limits resulting from chromatographic dispersion. The LC speciates the organotins and resolves spectral interferences from the analytes. A rapid method for extracting 97  $\pm$  or -8% of the TBT present in sediment into n-butanol is described. The detection limit is 3 ng/mL tin as TBT or 0.06 ng tin.

PB92-126499 PC A03/MF A01 National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Polymers Div.
Stability of Aqueous Inorganic Lead Solutions in

Polycarbonate Containers.

Annual rept. (Oct. 1991).

K. L. Jewett, W. R. Blair, F. E. Brinckman, and F. W. Wang. Dec 91, 27p NISTIR-4725

See also PB86-189875. Sponsored by Maryland Univ.

Keywords: \*Lead inorganic compounds, \*Liquids, \*Stability, \*Containers, Concentration(Composition), Water pollution, Monitoring, Acid treatment, Washing, Exposure, pH, Buffers(Cheinistry), Absorption, \*Lead acetate, Polycarbonates.

The stability of lead(II) acetate solutions at 50, 250 and 1000 mg/l (ppm as lead) in polycarbonate containers has been studied to assure reliable monitoring. The concentrations of aqueous solutions of lead maintained at pH 4.5 were determined at both short term (hours) and long term (months) exposures. Employing acid washed polycarbonate containers, no significant loss in lead concentration was detected for up to 100 hours after initial exposures to 50, 250 and 1000 ppm lead solutions. When containers were pretreated with lead solutions at comparable concentrations that would ultimately be contained within them, no significant loss in concentration was detected over more than 50 days.

PC A06/MF A02 PB92-126614 National Inst. of Standards and Technology, Gaithers-

Journal of Research of the National Institute of Standards and Technology, September-October 1991. Volume 96, Number 5.

1991, 65p

Also available from Supt. of Docs. as SN703-027-00042-3. See also PB92-126622 through PB92-126721 and PB92-110261. Library of Congress catalog card no. 89-656121.

Keywords: \*Research projects, \*Metrology, Dimensional measurement, Particle size, Microspheres, Dielectric properties, Permeability, Permittivity, Experimental design, Technology, Block design, Silicon isotopes, Voltametry, Air pollution detection, Dental caries, Chemical analysis, Sulfur dioxide, Carbon dioxide, Force standards, Standard reference materials, Orthogonal arrays, Advanced Technology Program, Isotope reference materials, Slovak Metrological Sociotope reference materials, Slovak Metrological Sociot

Contents: Summary of the Intercomparison of the Force Standard Machines of the National Institute of Standards and Technology, USA, and the Physika-lisch-Technische Bundesanstalt, Germany, Accurate and Precise Coulometric Determination of Sulfur Dioxide in Compressed Gas Mixtures; Development of a Coulometric Method for Assessing the Concentration of Ambient Levels of CO2/Air in Compressed Gas Mixtures; Certification of NIST SRM 1961--30 micrometers Diameter Polystyrene Spheres; Optimization Techniques for Permittivity and Permeability Determination; Taguchi's Orthogonal Arrays Are Classical Designs of Experiments; A Mathematical Model for Dental Caries--A Coupled Dissolution-Diffusion Process; The Advanced Technology Program--A New Role for NIST in Accelerating the Development of Commercially Important Technologies; A List of New Group Divisible Designs; Silicon Reference Materials Certified for Iso-tope Abundances; Slovak Metrological Society.

PB92-126713

(Order as PB92-126614, PC A06/MF A02) National Inst. of Standards and Technology, Gaithers-

burg, MD. Silicon Reference Materials Certified for Isotope

Abundances.
S. Valkiers, P. De Bievre, G. Lenaers, and H. S. Peiser. 1991, 3p Prepared in cooperation with Commission of the Euro-

pean Communities, Geel (Belgium). Central Bureau for Nuclear Measurements, and Antwerp Univ., Wilrijk (Belgium). Dept. of Chemistry. Included in Jnl. of Research of the National Institute of

Standards and Technology, v96 n5 p617-619 Sep/Oct

Keywords: \*Silicon isotopes, Silicon tetrafluoride, Mass spectroscopy, Atomic weights, \*Isotope reference materials, \*Reference materials, Isotope abun-

In a series of gas mass-spectrometric measurements performed near the highest attainable accuracy, samples from two highly homogeneous batches of silicon crystals and silica powder were compared directly with a synthetic mixture of the three stable isotopes of sili-con. Thereby, this work not only established the 'absolute' atomic weight of these batches, but also makes portions of these batches available as an Isotopic Reference Material for accurate isotopic abundance measurements in geochemical and other isotope-abundance studies of silicon.

PB92-127315 Not available NTIS Teknekron Sensor Development Corp., Menlo Park,

Opportunities for Innovation: Chemical and Blological Sensors.

M: Madou, and J. P. Joseph. Oct 91, 145p NIST/ GCR-91/593-1

Grant NANB9D0980 See also PB91-107078. Sponsored by National Inst. of Standards and Technology, Gaithersburg, MD.
Paper copy only available from National Institute of Standards and Technology, Gaithersburg, MD.

Keywords: \*Chemicals, \*Biological detection, \*Detectors, Technology transfer, Businesses, Markets, Solid state electronics, Measurement, Protons, Carbon dioxide, Machining, Semiconductors, Metal oxides, Gas detectors, Acoustic detectors, Improvement, Signal to noise ratio, Monitoring, Metabolin, Microsensors, Amperometric detectors.

Contents:

Application of Micromachining in Solid-State Chemical Sensors; The Challenges and Opportunities of Sensor

Technology; Metal Oxide Semiconductor Sensors; Amperometric Gas Sensors; Opportunities with Acoustic Sensors; Oxygen, Glucose, Urea, and Cholesterol Sensors for Biomedical Application; Biological Applications of Electrolyte/Insulator/ Silicon Structures;

and Market Introduction Issues for Chemical Microsensors.

#### **Basic & Synthetic Chemistry**

100.215

monds, \*Chemical.

AD-A243 094/0 PC A03/MF A01 National Inst. of Standards and Technology, Gaithers-

Determination of the Optical Constants of Thin Chemical-Vapor-Deposited Diamond Windows from 0.5 to 6.5 eV.

Technical rept. L. H. Robins, E. N. Farabaugh, and A. Feldman. 27 Sep 91, 19p Contract N00014-90-F-0011

Keywords: Absorption, Absorption spectra, Adsorption, Carbon, Chemicals, Constants, Energy, Etching, Fittings, Light scattering, Low energy, Models, Near ultraviolet radiation, \*Optical properties, Photons, Reflectance, Refractive index, Regions, Removal, Silicon, Single crystals, Substrates, Surfaces, Thinness, Transmittance, \*Chemical vapor deposition, \*Dia-

The optical constants of thin chemical-vapor-deposited diamond windows were determined as a function of photon energy from 0.5 to 6.5 eV by fitting experimental transmittance and a reflectance data to model that includes the effects of surface optical scatter. Rootmean-squared surface roughness values were also obtained from the analysis. The windows were fabriobtained from the analysis. The windows were fabri-cated by microwave plasma assisted CVD on silicon substrates, followed by partial removal of the sub-strates by etching. The values of the refractive index were diamonds. Substantial adsorption was found to occur in the visible to near ultraviolet region (2 to 5 eV) where single-crystal diamond is transparent. The spectrum of the low-energy absorption spectrum is dia-mond like amorphous carbon. There is a steep increase in absorption above the indirect bandgap of diamond (5.5 eV).

100,216

PB91-147447 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Ionizing Radiation Div.

Mechanism of OH Radical Reactions with Thymine and Uracil Derivatives.

Final rept.

S. V. Jovanovic, and M. G. Simic. 1986, 5p Pub. in Jnl. of the American Chemical Society 108, n19 p5968-5972 1986.

Keywords: \*Uracils, \*Thymine, \*Oxidation reduction reactions, \*Hydroxyl radicals, Chemical radicals, Oxidizers, Nucleotides, Radiolysis, Glycols, Pyrimidines, Reprints.

Yields of reducing, 6-yl, oxidizing, 5-yl, and methyl radicals, generated by OH radical reaction with uracil, thymine and 1-methyluracil, were determined by pulse radiolysis in aqueous solutions at pH 7. The absolute yields and ratio of 5-yl/6-yl radicals in uracil (20% 5-yl-U and 80% 6-yl-U) are altered in methyl substituted derivatives of uracil. For thymine one finds 35% of 5-ylderivatives of uracii. For inymine one finds 35% of 5-yi-1 and 57% of 6-yi-1, and for 1-methyluracii 20% of 5-yi-1-MeU and 65% of 6-yi-1-MeU radicals. The yields of pyrimidine glycols in the presence of an oxidizing agent (G = 3.2 for thymine glycols; 4.3 for uracii glycols; and 3.7 for 1-methyluracii glycol), as measured by HPLC, were shown to be equal to the yields of 5-OH-6-yl-Py reducing radicals of thymine (56% OH), uracil (80% OH) and 1-methyluracil (65% OH). It is suggested that 5-hydroxy-6-yl radicals are the exclusive pre-cursors of glycols. Mechanisms of glycol formation in the presence and absence of oxidizing agents are proposed and discussed.

#### 100.217

Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Chemical Kinetics Div.

#### CHEMISTRY

#### **Basic & Synthetic Chemistry**

Redox Reactions of Osmium Porphyrins.

Final rept.

S. Mosseri, P. Neta, D. Y. Sabry, P. Hambright, and

O. Mosself, T. Heid, D. T. Gably, T. Halliongth, and A. Harriman. 1988, 7p Pub. in Jnl. of the Chemical Society - Dalton Transactions 11, p2705-2711 1988.

Keywords: \*Osmium, \*Porphyrins, \*Oxidation reduction reactions, Photolysis, Radiolysis, Electrochemistry, Complex compounds, Ligands, Chemical reactions Register. tions, Reprints.

Cyclic voltammetric, gamma radiolytic, chemical and photochemical studies have shown that the metal centre in osmium porphyrine (OsP) can exist in a wide range of oxidation states, each being stabilized by axial complexation with a particular ligand. Thus, Os(II)P is stabilized by ligation with a CO molecule. Oxidation occurs readily to form the corresponding Os(III)P which retains the CO ligand and can be reduced quantitatively to the original Os(II) complex. Further oxidation can be achieved at hipper oxidant conther oxidation can be achieved, at higher oxidant con-centration, and the resultant Os(IV)P is stabilized by axial ligation of two alcohol or water molecules. These axial ligation to two action of water inforcules. These OS(IV) complexes are stable to both oxidation and reduction. Treating the OS(II)P with an organic peroxide results in formation of an OS(VI)P which is stabilized by two oxo ligands but can be reduced to the OS(VI)P. Photolysis of OS(II)P and OS(III)P causes loss of the CO ligand, the naked porphyrin species so formed un-dergoes oxidative reactions with the solvent, O2 or trace impurities, in most cases forming an Os(IV)P. Photolysis of Os(II)P in benzene containing small amounts of O2 generates the di-oxo Os(VI)P.

100,218 PB91-174730 PB91-174730 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Organic Analytical Research Div.

Oxidation of Organic Compounds by Active Manganese Dioxide.

Pub. in Organic Syntheses by Oxidation with Metal Compounds, Chapter 3, p119-260 1986.

Keywords: \*Manganese oxides, \*Oxidation, \*Alcohols, \*Amines, \*Hydrazines, Chemical reactivity, Chemical reactions, Reviews, Organic compounds, Reprints.

The recent, synthetic developments in the oxidation of organic compounds by active manganese dioxide has been reviewed. The topics covered are: (1) methods of preparation of active manganese dioxide; (2) aspects of mechanisms of oxidation by active manganese dioxide; an overview also includes (a) oxidation of alcohols and hydroxy compounds, (b) dehydrogenation and oxidative aromatization, (c) oxidation of hydrocarbons, (d) oxidation of amines and hydrazines, and (e) miscellaneous oxidations.

100,219 PB91-175125

Not available NTIS National Inst. of Standards and Technology (IMSE),

Gaithersburg, MD. Polymers Div.

Ion Incorporation into Octacalcium Phosphate Hydrolyzates. Final rept.

B. B. Tomazic, I. Mayer, and W. E. Brown. 1991, 13p Sponsored by American Dental Association Health Foundation, Chicago, IL.

Pub. in Jnl. of Crystal Growth 108, p670-682 1991.

Keywords: \*Calcium phosphates, Chemical analysis, Binary system(Materials), Crystal growth, Nonmetaliferous minerals, Aqueous solutions, Hydrolysis, Ions, Alkali metal compounds, Apatites, Spectroscopy, Solubility, Reprints.

There is considerable evidence indicating that biominerals are formed by precipitation of octacalcium phosphate followed by its hydrolysis. Therefore, the hydrolysis of octacalcium phosphate was studied in aqueous solutions of alkali nitrates/chlorides or carbonates. The hydrolysis was accompanied by incorporation of alkali and carbonate ions into apatite hydrolysis products. These were characterized by chemical analyses, infrared and X-ray diffraction spectroscopy, and solubility measurements. The extent of hydrolysis in carbonate-free media paralleled the extent of ion incorpo-ration: Li > Na > K. The hydrolyses in corresponding carbonate media produced less crystalline apatitic products with B-type carbonate substitution.

100,220 PB91-184853

PC A07/MF A01

National Inst. of Standards and Technology, Gaithersburg, MD.

Journal of Research of the National Institute of Standards and Technology. January-February 1991. Volume 96, Number 1.

1991, 150p Also available from Supt. of Docs as SN703-027-000-38-5. See also PB91-184861 and PB91-167411.

Keywords: \*Iron complexes, \*Iron organic compounds, \*Ceramics, Data bases, Calibrating, US NBS, Research projects, Stereo chemistry, Chirality, Carbenes, Biochemistry, Synthesis(Chemistry), Enantiomorphs, Reviews, High-TC superconductors.

Contents: New Chemical and Stereochemical Applications of Organoiron Complexes; International Conference on the Chemistry of Electronic Ceramic Materials; News Briefs; Calibration Services; Standard Reference Data.

100.221 PB91-184861

(Order as PB91-184853, PC A07/MF A01) National Inst. of Standards and Technology, Gaithersburg, MD.

New Chemical and Stereochemical Applications of Organoiron Complexes.
A. J. Fatiadi. 1991, 113p
Included in Jnl. of Research of the National Institute of

Standards and Technology, v96 n1 p1-113 Jan-Feb

Keywords: \*Iron complexes, \*Iron organic compounds, \*Chirality, \*Biochemistry, Reviews, Synthesis(Chemistry), Enantiomorphs, Carbenes, Synthesis(Chemistry), Enantiomorphs, Carbenes, Stereochemistry, Catalysts, Norbornadiene, Cycloal-Enantiomorphs, kanes, Porphyrins, Carbonyls, Ferrocene, Alkaloids.

The objective of the review is to provide a current overview of the rapidly developing chemistry of organometallic complexes and particularly organoiron complexes useful in asymmetric and stereoselective reactions. Also covered are stereoselective reactions of alpha, beta-unsaturated acyl ligands bound to the chiral auxiliary ((eta(sup 5)-C5H5) Fe(CO)(PPh3)) and new applications of organoiron complexes in the synthesis of natural products. The mechanistic aspects and stabilizing effects of the Fe(CO)3 group for alkenes or conjugated dienes are discussed. A brief summary of recent work on the special role of iron in biological reactions is also included.

PB91-237347 Not available NTIS

National Inst. of Standards and Technology (NML), Gaithersburg, MD. Ionizing Radiation Div. Antioxidation Mechanisms of Uric Acid. Final rept.

M. G. Simic, and S. V. Jovanovic. 1989, 5p Pub. in Jnl. of the American Chemical Society 111, n15 p5778-5782 1989.

Keywords: \*Uric acid, \*Oxidation reduction reactions, \*Reaction kinetics, Radiolysis, Antioxidants, Free radicals, DNA repair, Reprints.

One-electron oxidation of uric acid generates the urate radical which was studied in aqueous solution by pulse radiolysis and oxygen uptake measurements. Acid-base properties of the radical were determined, i.e., pKa1 = 3.1 + or - 0.1 and pKa2 = 9.5 + or - 0.1. The pra1 = 3.1 + 61 - 0.1 and pra2 = 9.5 + 01 - 0.1. The reaction of the radical with oxygen was too slow to be measured, k < 0.01dm2/mol/s. The one-electron redox potential vs. NHE, E7 = 0.59 V, was derived from the pH dependence of the redox potential, which was fitted through the values measured at pH 7, 8.9 and previously determined at pH 13. Rapid reactions of uric acid with oxidizing species, peroxy radicals and the guanyl radical, were indicative of uric acid as a possible water soluble physiological antioxidant and repair agent of oxidative damage to DNA bases.

Not available NTIS
National Inst. of Standards and Technology (NML),
Gaithersburg, MD. Organic Analytical Research Div.
Synthesis of 3-Quinuclidinol-(18)O, Benzilic-d5
Acid, and 3-Quinuclidinyl-(18)O, Benzilate-d5.
Final rept.
L. T. Spiegoski, F. Milling. 100,223 PB91-237370

L. T. Sniegoski, E. White, and G. D. Byrd. 1989, 11p Pub. in Jnl. of Labelled Compounds and Radiopharma-ceuticals 27, n9 p983-993 1989.

Keywords: \*Synthesis(Chemistry), \*Isotopic labeling, \*Benzilic acid, Standards, Mass spectroscopy, Oxygen 18, Purity, Reprints, \*Quinuclidinol, \*Benzilic acid/(quinuclidinyl-ester), Bicyclooctanol/aza, Benzene acetic acid/hydroxy-phenyl.

Isotopically labeled analogs of 3-quinuclidinol (Q), benzilic acid (BA), and 3-quinuclidinyl benzilate (BZ), for use as internal standards for isotope dilution measurements and the labeled intermediate 3-quinuclidinone and methyl benzilate used in their production, were synthesized. The isotopic purities of the 1-azabicyclo (2.2.2) octan-3-18O-ol, alpha-hydroxy-alpha-phenyl-d5-benzenacetic acid, and 3-quinuclidinyl-(18)O benzilate-d5 were determined and the electron impact ionization mass spectrum was obtained for each.

#### Industrial Chemistry & Chemical **Process Engineering**

100 224 PB91-162008 Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Chemical Engineering Science Div. Small Scale Demand Type Neon Liquefaction Plant.

Final rept.
W. P. Dube, A. J. Slifka, R. M. Bitsy, L. L. Sparks, and K. B. Johnson, 1990, 5p
Pub. in Advances in Cryogenic Engineering, v35

p1797-1801 1990.

Keywords: \*Neon, \*Liquefied gases, \*Pilot plants, Liquid hydrogen, Cryogenics, Liquefaction, Cost analysis, Circulation, Design, Reprints.

Low temperature measurement of the thermal conduc-Low temperature measurement of the thermal conductivity of insulating materials is generally made using a boil-off calorimetry technique involving liquid hydrogen (LH2). Liquid neon (LNe) has nearly the same normal boiling point as LH2, but has a much larger heat of vaporization, allowing extended run times. In the past, the main drawback of using LNe has been its excessive cost; \$170.00 per liter versus \$1.50 per liter for LH2 (1989 prices). A neon liquefaction plant has been designed and constructed to capture, purify and refrigered. designed and constructed to capture, purify and refrigerate the neon boil-off from calorimetry experiments. Recycling the neon reduces operating costs to ap-proximately \$20 per liter. The system consists of a purification section, which removes air and other contaminants from the calorimetry boil-off, a heat exchanger, LNe and LH2 storage dewars and a fully automated control system. After purification, neon is liquified in the heat exchanger by LH2 flowing counter-currently through stainless steel cooling coils. Hydrogen flow is automatically adjusted to keep the neon at its normal saturation temperature, 27 K. The liquid neon is then stored in a dewar placed directly below the heat exchanger. A 5 watt Gifford-McMahon refrigerator provides cooling during extended storage or low-flow applications.

100 225 PB91-162164 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Building Environment Div. Visualization of Nucleate Flow Boiling for an R22/

R114 Mixture and Its Components.

Final rept. M. A. Kedzierski, and D. A. Didion. 1990, 17p Sponsored by Electric Power Research Inst., Palo Aİto, CA.

Pub. in Experimental Heat Transfer 3, p447-463 1990.

Keywords: \*Nucleate boiling, \*Refrigerants, Bubbles, Heat of vaporization, Heat transfer, Thermodynamics, Binary mixtures, Convection, Optical measurement, Suppressing, Reprints.

Visualization of bubble nucleation during forced-convective flow inside a horizontal, electrically heated quartz tube was done in order to establish a comparison of this phenomenon between refrigerant mixtures and their pure components. The specific phenomena investigated were the suppression of nucleation due to increased mass flow quality while holding all other conditions fixed, and the comparison of the nucleate activity of the binary mixture to the nucleate activity of the pure components. The fluids investigated were a 37.7 mol% R22/62.3 mol% R114 binary mixture and the individual components R22 and R114. These fluids were pumped through an abraded, electrically heated quartz tube. A 16-mm high-speed camera was used, at

## Industrial Chemistry & Chemical Process Engineering

7000 frames/s, to film the boiling process. Detailed measurements of bubble frequency and bubble size were possible at low pressures, allowing direct calculation of the latent heat load required to nucleate a single bubble. Further work is required to develop a method that ensures statistically sound bubble frequency measurements. However, the standard deviations of the bubble diameter measurements were acceptable. The films were used to visually demonstrate the suppression of nucleation with increase in quality for R114, R22, and an R22/R114 mixture. The films suggest that, for a given quality, R114 exhibits much more nucleation than either R22 or the mixture, while the amount of nucleation demonstrated by R22 and the mixture was comparable even though the mixture was mostly R114 by mole. Arguments using the latent heat of vaporization, the vapor density, and the liquid thermal conductivity have been made to explain the visual trends.

100,226 Not available NTIS PB91-162222 National Inst. of Standards and Technology (NML), Boulder, CO. Thermophysics Div.

New Wide Range Equation of State for Helium. Final rept. R. D. McCarty, and V. D. Arp. 1990, 11p

Pub. in Advances in Cryogenic Engineering 35, p1465-1475 1990

Keywords: \*Liquid helium, \*Equations of state, Superfluidity, Cryogenics, Accuracy, Reprints.

A new correlation and computer code have been developed for helium. The correlation covers the temperature range of 0.8 to 1500 K using two equations of state, one for superfluid helium and another for the normal fluid. The equation of state for the normal fluid is valid for temperatures between 2 and 1500 K and for pressures up to 2000 MPa. The new normal fluid equation of state achieves increased accuracy in some regions of pressure and temperature, but not in others. There are unique problems involved in the correlation of helium data which prevent obtaining the accuracies which are more easily obtained for the properties of other fluids. Only the normal fluid equations are given here.

PB91-174672 Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Chemical Engineering Science Div Thermal Conductivity of Evacuated Perlite at Low Temperatures as a Function of Load and Load History.

tory.
Final rept.
W. P. Dube, L. L. Sparks, and A. J. Slifka. 1991, 4p
Sponsored by National Aeronautics and Space Administration, Bay Saint Louis, MS. John C. Stennis Space

Pub. in Cryogenics 31, n3-6 Jan 91.

Keywords: \*Penlite, \*Thermal conductivity, \*Evacuating(Vacuum), Thermal cycling tests, Hystereconductivity, sis, Cryogenics, Insulation, Physical properties, Dewar flasks, Reprints, Mechanical loading.

Perlite, a powdered insulation, is commonly used in large cryogenic storage dewars. When these dewars are thermally cycled, the perlite in the evacuated space between the inner and outer vessels of the dewar experiences a changing mechanical load due to thermal expansion and contraction of the inner vessel. Thermal conductivity data were obtained using a boil-off calorimeter. The apparent thermal conductivity of evacuated perlite increases strongly with applied load. Hysteretic behaviour of the conductivity was observed when perlite was subjected to cyclic mechanical loading.

100.228

PB91-175463 Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Chemical Engineering Science Div. Overview of Facilitated Transport Membrane Sys-

Final rent R. D. Noble, C. A. Koval, and J. J. Pellegrino, 1989,

Pub. in Chemical Engineering Progress, p58-70 Mar 89.

Keywords: \*Membrane transport, Separation, Reviews, Reprints, \*Facilitated transport membrane systems

A review is presented of membrane separation systems which use a reversible chemical reaction to achieve higher selectivities and fluxes that would otherwise be obtainable. Sections describe the system configurations, modeling, theoretical considerations and industrial experience. The authors have also compiled a table of many of the solute and chemical reacting carriers which have been studied for applications in facilitated transport membrane systems.

100.229

PB91-195487 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Center for Chemical Engineering. Application of Laser Diagnostic Techniques for the Examination of Liquid Fuel Spray Structure. Final rept.

C. Presser, A. K. Gupta, H. G. Semerjian, and R. J. Santoro. 1990, 28p Pub. in Chemical Engineering Communications 90,

p75-102 1990.

\*Drops(Liquids), \*Kerosene, Keywords: \*Sprays, Swirling, Air flow, Light scattering, Reprints, \*Droplet sizing, Spray combustion, Doppler interferometry.

Results are presented on the spatial distribution of mean droplet size and number density obtained from a hollow cone kerosene spray, introduced into nonswirling and swirling flow fields. An ensemble light scattering technique, based on measurement of the polarization ratio, has been employed to determine local droplet characteristics in dense and dilute regions of the spray. The measurements are complemented with Lorenz-Mie calculations of the scattering characteristics for a polydispersion of droplets of different size and refractive index. The results reveal that the degree of swirl imparted to the surrounding air flow, has a strong influence on spray structure. For all conditions examined the mean droplet size is found to be larger on the spray boundary than towards the centerline. Mean droplet size is also found to increase with distance at all radial positions of the spray; this trend is attributed to the vaporization of smaller droplets and/ or possible coalescence between the droplets. In addition to the ensemble technique, measurements have also been obtained with the phase/Doppler interferometry and light intensity devonolution techniques under identical experimental conditions. The mean droplet sizes obtained with the ensemble approach are in general smaller than those measured with the phase/Doppler technique.

100.230

PB91-195719 Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Chemical Engineering Science Div Application of Osmotic Dewatering to the Con-trolled Crystallization of Biological Macromole-cules and Organic Compounds.

Final rept. P. Todd, S. K. Sikdar, C. Walker, and Z. R. Korszun. 1991, 10p Pub. in Jnl. of Crystal Growth 110, p283-292 1991.

Keywords: \*Lysozyme, \*Crystallization, \*Dewatering, Crystallography, Proteins, Transport properties, Reprints, \*Reverse osmosis.

Several methods of crystallization of biological macromolecules depend upon the transport of water through the vapor phase - a process that is sensitive to ambient conditions (temperature, relative humidity). Other methods depend on the transport of solute by diffusion or through a membrane. By regulating the solute concentration on the outside of a reverse-osmosis mem-brane it is possible to control the rate at which macromolecules and other solutes are concentrated inside a membrane-bound fluid. The effect of dewatering rate on lysozyme crystal quality and growth rate was assessed. A 3-fold increase in concentration over a 9 day period yielded tetragonal crystals 0.5 mm on a side with sharp edges and with ordering at least to 1.73 A. Transparent crystals of triglycine sulfate were grown by osmotic dewatering; in this case crystal growth could be enhanced or reversed by manipulating the external solution.

100,231

PB91-237230 Not available NTIS National Inst. of Standards and Technology (CSTL), Boulder, CO. Chemical Engineering Div.

Electrokinetic Demixing of Two-Phase Aqueous Polymer Systems. 2. Separation Rates of Polyethyleńe Glycól-Maltodextrin Mixtures. Final rept

K. S. M. S. Raghava Rao, R. M. Stewart, and P. W. Todd. 1991, 11p See also Part 1, PB91-159095

Pub. in Separation Science and Technology 26, n2 p257-267 1991

Keywords: \*Separation processes, \*Solvent extraction, \*Electrophoresis, \*Dextrin, Binary system(Materials), Polyoxyethylene, Electrokinetics, Aqueous solutions, Proteins, Electric fields, Buffers(Chemistry), Polarity, Temperature dependence, Phosphates, Biochemistry, Reprints.

A method for enhanced demixing of agueous twophase systems in a thermostated vertical electrophoresis column was therefore studied. The effects of the electric field strength, field polarity, temperature, phase composition, and buffer concentration on demixing rates of a polyethylene glycol-maltodextrin (PEG-MDX) system were quantitatively measured. At normal electrical polarity (anode at the top of the column), using a maximum practicable field strength of 26.4 V/cm, the demixing rate was twice that in zero electric field at 25 + or - 2 C. With polarity reversed (anode at the bottom, electric field opposing gravitational settling) at a field of 26.4 V/cm, demixing was 5.5 times as fast as in zero field. Reduction of the temperature from 25 to 14 C caused an increase in demixing rate in the absence of an applied field, while reduced temperature did not change the rate when using electric fields of either normal or reverse polarity. Increased phosphate buffer concentration substantially increased the demixing rate for PEG-MDX mixtures.

100,232

PB91-237297 Not available NTIS National Inst. of Standards and Technology (CSTL), Gaithersburg, MD. Thermophysics Div.

Thermodynamics of Solutions Near the Solvent's Critical Point.

Final rept. J. M. H. Levelt Sengers. 1991, 56p Pub. in Supercritical Fluid Technology: Reviews in Modern Theory and Applications, Chapter 1, p1-56

Keywords: \*Fluids, \*Solutions, \*Critical point, Helmholtz free energy, Dilution, Solvents, Thermodynamics, Reprints, Supercritical solubility, Near critical fluids.

This chapter gives a description of dilute-mixture critical behavior that is aimed at the practicing chemical engineer. The basic concepts of critical behavior in pure fluids and fluid mixtures are explained with a maximum of practical examples and graphical material. Many of the peculiarities of dilute near-critical mixtures are described by means of a simple power-series expansion of the classical mixture Helmholtz free energy. Attention is given to the sources of increased error in experiments carried out in near-critical fluids. A number of misleading statements about supercritical solubility that have recently occurred in the literature are reviewed and corrected.

100.233

PB91-237578 Not available NTIS National Inst. of Standards and Technology (CSTL), Gaithersburg, MD. Thermophysics Div. Thermodynamic Properties of 1,1,1,2,-Tetrafluor-

oethane (R134a) in the Critical Region.

Final rept. S. Tang, G. X. Jin, and J. V. Sengers, 1991, 26p

Contract DE-FG05-88ER13902 Sponsored by Department of Energy, Washington, DC. Pub. in International Jnl. of Thermophysics 12, n3 p515-540 May 91.

Keywords: \*Fluorohydrocarbons, \*Equations of state, \*Critical point, \*Thermodynamic properties, Refrigerants, Temperature dependence, Specific heat, Acoustic velocity, Reprints, 1 1 1 2-Tetrafluoroethane(R134a).

A theoretically based simplified crossover model, which is capable of representing the thermodynamic properties of fluids in a large range of temperatures and densities around the critical point, is presented. The model is used to predict the thermodynamic properties of R134a in the critical region from a limited amount of available experimental information. Values for various thermodynamic properties of R134a at den-

#### **CHEMISTRY**

## Industrial Chemistry & Chemical Process Engineering

sities from 2 to 8 mol/L and at temperatures from 365 to 450 K are presented.

Photo & Radiation Chemistry

AD-A227 868/7 PC A02/MF A01 National Inst. of Standards and Technology, Gaithersburg, MD.

Laser Photolysis of Trimethylgallium at 193 nm: Quantum Yields for Methyl Radical and Ethane Production.

W. Braun, R. Klein, A. Fahr, H. Okabe, and A. Mele. 2 Mar 90, 8p ARO-25911.1-CH, Contract MIPR-119-89

Pub. in Chemical Physics Letters, v166 n4 p397-403, 2 Mar 90.

Keywords: Chemical reactions, Ethanes, Gallium, Lasers, Methyl radicals, \*Photolysis, Production, Quantum efficiency, Reprints, Vapor deposition, Yield, Organic chemistry, \*Gallium organic compounds, Isotopic labeling.

Quantum yields for the products from trimethylgallium (TMG) photolysis were determined via a new method involving isotopic analysis using TMG-acetone-d6 mixtures. The following model-dependent quantum yields were obtained: monomethylgallium (MMG), 0.5; dimethylgallium (DMG), 0.2; gallium, 0.3; molecularly eliminated ethane, 0.3; free methyl, 1.5. Two new electronic absorptions at 216 and 220 nm were found and are tentatively ascribed to DMG. Keywords: Trimethylgallium, Quantum yield, Laser photolysis, Chemical vapor deposition, Reprints. (JS)

100,235

PB91-147066 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Surface Science Div.

Laser Induced Desorption of Molecules from Surfaces.

Final rept.

R. R. Cavanagh, S. A. Buntin, L. J. Richter, and D. S.

King. 1990, 12p Sponsored by Department of Energy, Washington, DC. Pub. in Comments on Atomic and Molecular Physics 24, n6 p365-376 1990.

Keywords: \*Surface reactions, Photochemical reactions, Excitation, Heating, Reprints, \*Laser induced de-

Great insight into the fundamental mechanisms of opti-cally driven surface processes has been obtained through studies of laser induced desorption of species from well characterized surfaces in ultrahigh vacuum. Key fundamental studies are reviewed, with emphasis placed on three distinct processes by which photons can promote surface reactions: heating, resonant adsorbate excitation, and substrate electronic excitation.

PB91-147793 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Chemical Kinetics Div. Radiation Chemistry of Enones.

Final rept.

P. Neta, and M. Dizdaroglu. 1989, 24p Sponsored by Department of Energy, Washington, DC. Pub. in Chemistry of Enones, Chapter 16, p757-780 1989

Keywords: \*Aldehydes, \*Detones, \*Radiation chemistry, Ionizing radiation, Solutions, Chemical radicals, Reviews, Radiolysis, Reprints.

Radiation chemistry deals with the chemical effects of ionizing radiation, such as X-rays, gamma rays, high energy electrons, or other energetic particles. Ionizing radiation is absorbed in organic materials somewhat indiscriminately and causes ionizations and excitations which may result in bond scission. In discussing the radiation chemistry of an organic compound, the au-thors distinguish between the radiation chemistry of the neat compound, where the energy is absorbed to-tally by the compound itself, and the radiation chemis-try of its solutions, where the energy is absorbed predominantly by the solvent. In the latter case, the solute undergoes chemical changes only via reactions with the primary radicals formed from the solvent. The radiation chemistry of enones was studied mainly in solution, as will become clear from the review, and most often it involved aqueous solutions.

PB91-148809 Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Quantum Physics Div.

Novel Laser Gain and Time-Resolved FTIR Studies of Photochemistry.

Final rept.

S. R. Leone. 1989, 13p Contract DAAG-29-85-K-0033, Grant NSF-CHE84-08403

Sponsored by Department of Energy, Washington, DC., and National Science Foundation, Washington, DC

Pub. in Proceedings of International Conference on Laboratory Research for Planetary Atmospheres (1st), Bowie, MD., October 25-27, 1989, p129-141.

Keywords: \*Planetary atmospheres, \*Cometary atmospheres, \*Photochemical reactions, Infrared spectra, Emission spectra, Acetylene, Tunable lasers, Reprints. Fourier transform infrared spectroscopy.

Several novel techniques are discussed which can be used to explore laboratory photochemical processes and kinetics relevant to planetary atmospheres; these include time-resolved laser gain-versus-absorption spectroscopy and time-resolved Fourier transform infrared (FTIR) emission studies. The laser gain-versus-absorption method employs tunable diode and Fcenter lasers to determine the yields of excited photo-fragments and their kinetics. The time-resolved FTIR technique synchronizes the sweep of a commercial FTIR with a pulsed source of light to obtain emission spectra of novel transient species in the infrared. These methods are presently being employed to investigate molecular photodissociation, the yields of excited states of fragments, their subsequent reaction kinetics, Doppler velocity distributions, and velocity-changing collisions of translationally fast atoms. Such techniques may be employed in future investi gations of planetary atmospheres, for example to study polycyclic aromatic hydrocarbons related to cometaryemissions, to analyze acetylene decomposition products and reactions, and to determine spectral features in the near infrared and infrared wavelength regions for planetary molecules and clusters.

100,238

PB91-149252 Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Quantum Physics Div. Periodic Orbits and Diffuse Structures in the Pho-

todissociation of Symmetric Triatomic Molecules. Final rept.

R. Schinke, and V. Engel. 1990, 5p Pub. in Jnl. of Chemical Physics 93, n5 p3252-3256, 1 Sep 90.

Keywords: \*Photodissociation, Triatomic molecules, Trajectories, Orbits, Reprints.

The authors reinvestigate the collinear photodissociation of a symmetric triatomic molecule studied a decade ago by Kulander and Light (J. Chem. Phys. 73,4437 (1980)), within the time-dependent formalism. The diffuse structures in the absorption spectrum are uniquely related to three, well separated recurrences which, in turn, are explained by three generic periodic orbits of the corresponding classical Hamiltonian. One of these orbits describes pure symmetric stretch motion while the other two orbits combine symmetric stretch and hyperspherical motion. The applicability of simple one-dimensional, zeroth-order pictures is reviewed in the light of these new results.

100.239

PB91-149260 Not available NTIS National Inst. of Standards and Technology (NML),

Boulder, CO. Quantum Physics Div.
Photodissociation of C(I)NO in the S(I)State: A
Quantum-Mechanical ab initio Study.

R. Schinke, M. Nonella, H. U. Suter, and J. R. Huber. 1990, 9p

Pub. in Jnl. of Chemical Physics 93, n2 p1098-1106, 15

Keywords: \*Photodissociation, Absorption spectra, Vibrational states, Rotational states, Quantum mechanics, Nitric oxide, Potential energy, Reprints, \*Nitrosyl chloride.

The authors investigated the photodissociation of CINO (nitrosyl chloride) via the S(1) electronic state using a three-dimensional (3D) ab initio potential-energy surface (PES). The dissociation is found to be fast and direct. In the Franck-Condon (FC) region the slope of the potential along the dissociation path is relatively small giving rise to narrow partial absorption peaks. The total absorption spectrum therefore exhibits a broad vibrational structure which is in perfect agreement with recent measurements. The vibrational excitation of the NO fragment is small and can be qualitatively described within the adiabatic approximation. It is found to be very sensitive to the vibrational FC factor in the transition region. The rotational state distribution of NO is highly inverted with a peak around j=30. It is readily explained by the rotational reflection principle. The experimental results are satisfactorily reproduced by the authors' calculations which underlines the overall quality of the calculated PES. Minor adjustments are necessary, however, to quantitatively reproduce the vibrational branching ratio.

100,240

PB91-203679 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Chemical Kinetics Div. Mechanism of Cyanide Release in the Radiolysis

of Acetonitrile.

Final rept. S. Mosseri, P. Neta, and D. Meisel. 1990, 5p Pub. in Radiation Physics and Chemistry 36, n6 p683-687 1990.

Keywords: \*Acetonitrile, \*Cyanides, \*Radiolysis, Chemical reactions, Chemical radicals, Peroxy radicals, Solutions, Reprints.

The radiolysis of neat acetonitrile or of its aqueous solutions was found to lead to formation of cyanide ions, but only in the presence of oxygen. The mechanism involved formation of the acetonitrile radical, (dot)CH2CN, which reacts with O2 to give the peroxyl radical, NCCH2O2(dot). Subsequent decay of the peroxyl radical results in the release of HCN. From the yield of cyanide under various conditions the authors conclude that the peroxyl radicals decay via two main routes, the products of one route from cyanide directly while the product of the second route yield cyanide only after hydrolysis by alkali. The overall yield of CN(-) in 5% acetonitrile aqueous solutions saturated with a mixture of N2O:02 (4:1) was G approximately equal to 6 in alkaline solution and G approximately equal to 1 in neutral solution. The yield of CH2O in both solutions was G approximately equal to 1.5.

100.241

PB91-236489 Not available NTIS National Inst. of Standards and Technology (PL), Gaithersburg, MD. Ionizing Radiation Div. Mechanisms of the Reduction Reactions of Cr(VI)

in the Radiolysis of Acidic Potassium and Silver Di-chromate Solutions in the Presence or Absence of

Acetic Acid. Final rept. M. Al-Sheikhly, and W. L. McLaughlin. 1991, 9p Pub. in Radiation Physics and Chemistry 38, n2 p203-

Keywords: \*Chromates, \*Oxidation reduction reactions, \*Reaction kinetics, \*Acetic acid, Silver ions, pH, Radiolysis, Chemical dosimeters, Chemical radicals, Computerized simulation, Reprints, Radiation chemical mechanisms.

The mechanisms and the kinetics of reactions in deoxygenated and oxygen-saturated aqueous solutions of potassium dichromate in the range of pH 0.4-0.8, in the presence and absence of acetic acid, were investigated by pulse and steady-state radiolysis. Computer simulation of reaction mechanisms was compared with exulation of reaction mechanisms was compared with experimental kinetics data for solutions containing silver dichromate and acetic acid. It was found that carboxymethyl reduces Cr(VI) to Cr(V) with a rate constant of 1.8 x 10 to the 8th power/M/s, while carboxymethlyperoxyl does not reduce Cr(VI). Hydroperoxyl reduces Cr(VI) to Cr(V), but at a much lower rate constant of < 10 to the 6th. The oxidation-reduction reaction between radiolytically produced Cr(V) and Ag(II) was measured and found to have a rate constant of 1.0 x 10 to the 8th power/M/s. The mechanisms for the en-10 to the 8th power/M/s. The mechanisms for the enhanced stability of Cr(VI) in the presence of Ag+ was studied in the light of the kinetics and the reactivity of the Ag(II) with the intermediate free radicals occurring in this system. The present findings help elucidate the

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mechanisms of the dichromate dosimeter, its doserate independent response and its stability.

# **Physical & Theoretical Chemistry**

AD-A227 296/1 PC A04/MF A01 National Inst. of Standards and Technology, Boulder, CO.

Detection of Excited States by Laser-Induced Flu-orescence and Analysis of Energy Transfer.

Final rept. Oct 88-Sep 89.

J. Borysow, and A. V. Phelps. Sep 90, 70p WRDC-TR-90-2081,

Contract MIPR-FY-88-N0655

Keywords: Absorption, Collisions, Detection, Diodes, Doppler effect, Electric fields, Energy, Energy transfer, Field intensity, Impact, Ionization, Kinetic energy, \*Laser induced fluorescence, Lasers, Measurement, Nonlinear systems, Profiles, Pulses, Rotation, Time dependence, \*Nitrogen ions, \*Excited states, Gas ionization. ization.

The laser absorption technique was improved through the use of laser diodes and was applied to absorption measurements of the line profiles for the A2 pi u from x 2 sigmag(+) transition of N2(+) ions to determine (a) the electric field strength in the positive column of pulsed discharges in N2 from the Doppler shift and broadening, (b) the time dependence of the density of ground state N2(+) ions drifting through N2 resulting from the transfer of kinetic energy of the N2(+) to rotational energy. An analysis of the impact of measurements made under this program on models of nonlinear ionization in N2 leads to the conclusion that ionization by collisions between pairs of metastable N2 molecules in the a' state probably make the largest contribution to the growth of instabilities in high-current discharges. (RH)

AD-A228 082/4 PC A02/MF A01 National Inst. of Standards and Technology, Gaithersburg, MD.

Vibrational Spectra of Molecular Ions Isolated in

Solid Neon. III. N4(+).

W. E. Thompson, and M. E. Jacox. 15 Sep 90, 8p ARO-25664.4-CH, Contract MIPR-120-90

Pub. in Jnl. of Chemical Physics, v93 n6 p3856-3862. 15 Sep 90.

Keywords: Absorption, Atoms, \*Electron spin resonance, Infrared radiation, Infrared spectra, Intensity, Microwaves, \*Molecular ions, Neon, Solids, \*Vibrational spectra, Nitrogen.

When a Ne:N2=100 or 200 mixture is codeposited at 5 K with a beam of neon atoms excited by a microwave discharge, a weak to moderately intense infrared absorption appears at 2237.6 cm-1 which is assigned to the N4 molecular ion. The analysis of the infrared spectra of the nitrogen-15 substituted species of N4 supports the conclusion from earlier ab initio calculations and electron spin resonance observations that N4 has a linear, centrosymmetric ground-state structure. For the N4 species with noncentrosymmetric isotopic substitution, the in-phase end-atom stretching fundamental becomes infrared active and has also been observed. Although the anion responsible for overall charge neutrality of the deposit has not been definitively identified, secondary photolysis studies provide some information regarding its properties. (js)

100.244 AD-A230 957/3 PC A03/MF A01 National Inst. of Standards and Technology (NML), Gaithersburg, MD. Molecular Physics Div. Vibrational Spectra of Molecular Ions Isolated in Solid Neon. IV.NO(+), NO(-), ONNO(+), and ONNO(-).

M. E. Jacox. 1 Dec 90, 14p ARO-25664.7-CH, Contract ARO-MIPR-120-90

Pub. in Jnl. of Chemical Physics, v93 n11 p7609-7621, 1 Dec 90

Keywords: Absorption, Atoms, Dimers, Electrons, Infrared radiation, Ionization, Ions, Molecular ions, Neon, Photoionization, Solids, Stabilization, Vibrational spectra, Reprints, \*Vibrational spectra, \*Neon.

When a Ne:NO sample is codeposited at approximately 5 K with a beam of neon atoms that has been excited in a microwave discharge, photoionization and Penning ionization of the NO leads to the stabilization of both monomer and dimer ions. The most prominent infrared absorption, at 1619.2 cm-1, results from the reaction of NO- with No or of an electron with (NO)2 to form the charge-delocalized trans-ONNO- species. The position of the totally symmetric NO-stretching absorption of trans-ONNO- can be inferred from observation of a combination band. The infrared absorption of NO+ has been detected very close to the gas-phase band center. Other infrared absorptions have been tentatively assigned to NO-, cis-ONNO-, trans-ONNO, and the lowest energy isomer of ONNO+. Comparison of the gas-phase vibrational frequencies observed for the weakly bound species cis-ONNO and N2O3 with the corresponding frequencies observed in this neon-matrix study suggests that the matrix shifts for the dimer ion absorptions in the mid-infrared probably amount to less than 1%.

100,245

AD-A234 043/8 PC A03/MF A01 National Inst. of Standards and Technology (NML), Gaithersburg, MD. Molecular Spectroscopy Di

Production and Spectroscopy of Small Polyatomic Molecular Ions Isolated in Solid Neon. M. E. Jacox, and W. E. Thompson. 1990, 11p ARO-

25664.2-CH. Contract ARO-MIPR-120-90

Availability: Pub. in High Temperature Science, v28 p225-234 1990. Available only to DTIC users. No copies furnished by NTIS.

Keywords: Absorption, Spectroscopy, Neon, \*Molecular ions, Infrared spectra, Reprints, Molecular clusters, Cluster ions, \*Matrix isolation, Solidified gases.

No abstract available

100,246

AD-A235 490/0 PC A03/MF A01 National Inst. of Standards and Technology (IMSE), Gaithersburg, MD. Metallurgy Div.

Thermodynamic and Kinetic Stability of Refractory Materials at Ultra-High Temperatures.

Annual rept. 1 Oct 89-30 Sep 90. J. W. Hastie, P. K. Schenck, and D. W. Bonnell. Nov 90, 31p AFOSR-TR-91-0447, Grant AFOSR-ISSA-90-0026

Keywords: Equilibrium(General), Extrapolation, \*Hafnium compounds, Heat, High temperature, Kinetics, Lasers, Mass spectra, Measurement, Oxides, Pulsed lasers, \*Refractory materials, \*Silicon carbides, Stability, Surface temperature, Thermodynamics, Time, Vacuum, Vapor pressure, \*Vaporization, LVMS(Laser Vaporization Mass Spectrometry), Mass spectrometry, \*Thermal stability, Reaction kinetics, \*High temperature, \*Ceramic materials, Spectrum analysis, Reaction kinetics.

Using the newly developed measurement technique of Laser Vaporization Mass Spectrometry (LVMS), new vapor pressure data for hafnium oxide and alpha silicon carbide at ultra high temperature have been obtained. The technique uses pulsed lasers to heat a surface on the timescale of 15 ns, providing an effectively containerless environment. Time-resolved mass spectra establish that the vaporization process is occurring under at least local equilibrium conditions. The vapor pressure data are compared with extrapolations from the literature. The agreement for HfO2 is excellent, while the comparison for SiC indicates a significant discrepancy. Both instrumental and physio-chemical influences affecting the measurements are discussed, and the possibility of a different vaporization mechanism for SiC under vacuum vaporization conditions is suggested. Preliminary optical spectroscopic approaches, to supplement the current indirect methods, to the direct measurement of surface temperatures under short pulse laser heating conditions are present-

100.247

AD-A236 485/9 PC A03/MF A01 National Inst. of Standards and Technology, Gaithersburg, MD.

Spatially and Spectrally Resolved Cathodoluminescence of Hot-Filament Chemical-Vapor-Deposited Diamond Particles. Interim rept.

L. H. Robins, E. N. Farabaugh, and A. Feldman. 24 Apr 91, 43p

Contract N00014-90-F-0011

Keywords: Brightness, Broadband, Cathodoluminescence, Deposition, Impurities, Particles, Temperature, Carbon, \*Diamond, Crystal growth, Vapor deposition.

Spectrally resolved cathodoluminescence (CL) image and spatially resolved CL spectra were obtained from two specimens grown by hot-filament chemical vapor deposition. Each specimen consisted of a large number of unconnected diamond particles with cubo-octahedral and pseudo-five-fold twinned growth habits. The growth temperature was nominally 600 deg C for one specimen and 750 deg C for the other. In the 1.5-3.5 eV range, the spectra are composed of four defect and impurity related bands: there are three bands with zero-phonon lines at 1.68 eV, 2.156 eV, and 2.325 eV, and one broad band centered at 2.85 eV. A weak at 5.27 eV, due to exciton recombination, was also observed. Spectrally resolved images to the two most intense CL bands, at 2.126 eV and 2.85 eV, were obtained for several particles. In the low temperature specimen, bright regions in images of the 2.85 eV band are correlated in some cases with the central regions of (100) facets.

100,248 AD-A237 128/4 PC A03/MF A01 National Inst. of Standards and Technology (IMSE), Gaithersburg, MD. Ceramics Div.

Spatially and Spectrally Resolved Cathodoluminescence of Hot-Filament Chemical-Vapor-Deposited Diamond Particles.

Interim rept. L. H. Robins. 24 Apr 91, 40p Contract N00014-90-F-0011

Keywords: Broadband, \*Cathodoluminescence, Growth(General), Impurities, Particles, Temperature, \*Diamonds, Crystal growth, \*Vapor deosition.

Spectrally resolved cathodoluminescence (CL) image and spatially resolved CL spectra were obtained from two specimens grown by hot-filament chemical vapor deposition. Each specimen consisted of a large number of unconnected diamond particles with cubooctahedral and pseudo-five-fold twinned growth habits. The growth temperature was nominally 600 C for one specimen and 750 C for the other. In the 1.5-3.5 eV range, the spectra are composed of four defect and impurity related bands: there are three bands with zero-phonon lines at 1.68 eV, 2.156 eV, and 2.325 eV, and one broad band centered at 2.85 eV. A weak peak at 5.27 eV, due to exciton recombination, was also observed. Spectrally resolved images of the two most intense CL bands, at 2.156 eV and 2.85 eV, were obtained for several particles.

100.249 AD-A238 415/4 Not available NTIS National Inst. of Standards and Technology, Gaithersburg, MD.

Vibrational Spectra of Molecular Ions Isolated in

Wild Neon. 6. CO4(-).

M. E. Jacox, and W. E. Thompson. 4 Apr 91, 8p
ARO-25664.9-CH

Contract ARO-MIPR-120-90

Pub. in Jnl. of Physical Chemistry, v95 n7 p2781-2787, 4 Apr 91. Available only to DTIC users. No copies furnished by NTIS.

Keywords: Molecular spectroscopy, \*Molecular vibration, Carbonates, Carbon dioxide, Oxygen, Nitrogen, Reprints, \*Neon matrices, \*Vibrational spectra, \*Molecular ions.

No abstract available

100.250 AD-A239 729/7 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Molecular Physics Div. Vibrational Spectra of Molecular Ions Isolated in Solid Neon. 7. CO(+), C2O2(+), and C2O2(-). W. E. Thompson, and M. E. Jacox. 15 Jul 91, 11p ARO-25664.10-CH,

Pub. in Jnl. of Chemical Physics, v95 n2 p735-745, 15 Jul 91. Available only to DTIC users. No copies furnished by NTIS.

# Physical & Theoretical Chemistry

Keywords: \*Neon, \*Carbon monoxide, \*Ion molecule interactions, \*Infrared spectra, Photoionization, Ionized gases, Vapor deposition, Absorption, Atomic beams, Electron capture, Reprints, \*Molecular ions, Solids, \*Vibrational spectra, Penning ionization, Low temperature research.

No abstract available.

100.251 PB90-244526 Not available NTIS American Chemical Society, Washington, DC.
Journal of Physical and Chemical Reference Data, Volume 19, Number 1, 1990.

Quarterly rept. c1990, 319p See also PB90-244534 through PB90-244591 and PB90-161241. Prepared in cooperation with American Inst. of Physics, New York. Sponsored by National Inst. of Standards and Technology, Gaithersburg, MD. Available from American Chemical Society, 1155 16th St., NW, Washington, DC 20036.

Keywords: \*Magnesium oxides, Thermodynamic properties, Benzenes, Thermal conductivity, Standards, Atomic energy levels, Butanes, Reaction kinetics, Combustion, Periclase, Surface structure, Ion scattering, Aluminum ions, Iron ions, Oxygen atoms, Electronatom collisions, Isobutyl radicals, 2-methylpropane.

Contents: Chemical Kinetic Data Base for Combustion Chemistry. Part 4. Isobutane; Thermodynamic Func-tions and Properties of MgO at High Compression and High Temperature; Critical Compilation of Surface Structures Determined by Ion Scattering Methods; Benzene--A Further Liquid Thermal Conductivity Standard; Energy Levels of Atomic Aluminum with Hyperfine Structure; Spectral Data and Grotrian Diagrams for Highly Ionized Iron, Fe VIII-XXVI; Updated Excitation and Ionization Cross Sections for Floriton xcitation and Ionization Cross Sections for Electron Impact on Atomic Oxygen.

100.252 PB90-244534

(Order as PB90-244526)

National Inst. of Standards and Technology (NML), Gaithersburg, MD. Chemical Kinetics Div. Chemical Kinetic Data Base for Combustion Chemistry Part 4. Isobutane.

Quarterly rept. W. Tsang. c1990, 68p Contract DNA-001-85-C-0022

Sponsored by Defense Nuclear Agency, Washington,

Included in Jnl. of Physical and Chemical Reference Data, v19 n1 p1-68 1990. Available from American Chemical Society, 1155 16th St., NW, Washington, DC

Keywords: \*Butanes, \*Reaction kinetics, \*Combustion, Pyrolysis, Tables(Data), \*Isobutyl radicals, \*2-methylpropane, Data bases.

The publication contains evaluated and estimated data on the kinetics of reactions involving isobutane, t-butyl radical and isobutyl radical and various small inorganic and organic species which are of importance for the proper understanding of isobutane combustion and pyrolysis. It is meant to be used in conjunction with the tinetic data given in earlier publications, which is of direct pertinence to the understanding of methane, ethane, methanol and propane pyrolysis and combustion, but which also contains a large volume of data that are applicable to the isobutane system. The temperature range covered is 300-2500 K and the density range 1 x 10 to the 16 power to 1 x 10 to the 21 power molecules/cc. (Copyright (c) 1990 by the U.S. Secretary of Commerce.)

100.253 PB90-244542

(Order as PB90-244526)

California Univ., Los Angeles. Thermodynamic Functions and Properties of MgO at High Compression and High Temperature. Quarterly rept.

O. L. Anderson, and K. Zou. c1990, 15p Grants DOE-ER-13803, NSF-EAR86-17290 Sponsored by Department of Energy, Washington, DC., and National Science Foundation, Washington, DC.

Included in Jnl. of Physical and Chemical Reference Data, v19 n1 p69-84 1990. Available from American Chemical Society, 1155 16th St., NW, Washington, DC Keywords: \*Magnesium oxides, \*Thermodynamic properties, Gibbs free energy, Helmholtz free energy, Entropy, \*Periclase, High pressure, High temperature.

The complete thermodynamic functions for MgO (the mineral periclase) are presented for the temperature range 300-2000 K and the pressure range 0-150 GPa, both as tables and as graphs. Careful attention is given to the temperature and pressure dependence of the coefficient of thermal expansion alpha and the isothermal bulk modulus K(T), which are the major corrections to the thermodynamic functions in extreme conditions. The Birch-Murnaghan equation of state is used to account for certain terms in the expressions for internal energy and enthalpy. The parameters used in the Birch-Murnaghan equation of state are given as functions of temperature. The parameters which pres-ently limit the calculations of thermodynamic functions to even higher temperatures and pressures and limit the applications of this method to other minerals are

100,254 PB90-244559

(Order as PB90-244526)

Oregon State Univ., Corvallis. Dept. of Chemistry.
Critical Compilation of Surface Structures Determined by Ion Scattering Methods.
Quarterly rept.

P. R. Watson, c1990, 27p Grant NBS-60NANB7D0729

Sponsored by National Inst. of Standards and Tech-

Included in Jnl. of Physical and Chemical Reference Data, v19 n1 p85-112 1990. Available from American Chemical Society, 1155 16th St., NW, Washington, DC

Keywords: Crystal structure, Reviews, Comparison, \*Surface structure, \*Ion scattering, Low energy electron diffraction. Semiconductors.

The review critically compiles all surface structures derived by ion scattering techniques reported in the refereed literature prior to January 1988. They are compared with the more extensive low-energy electron diffraction database reported previously (J. Phys. Chem. Ref. Data 16, 953 (1957)). These investigations cover all types of surfaces including clean and adsorbate-covered metal semiconductor, and other nonmetallic covered metal, semiconductor, and other nonmetallic substrates. The important experimental and theoretical aspects of such investigations have been extracted into easily understood tabular form supplemented by many figures and ancillary tables and complete references. (Copyright (c) 1990 by the U.S. Secretary of Commerce.)

100,255 PB90-244567

(Order as PB90-244526) Thessaloniki Univ., Salonika (Greece). Benzene: A Further Liquid Thermal Conductivity

Quarterly rept.

Quarterly rept.
M. J. Assael, M. L. V. Ramires, C. A. Nieto de
Castro, and W. A. Wakeham. c1990, 3p
Contract DNA-001-85-C-0022
Sponsored by Defense Nuclear Agency, Washington,
DC., Lisbon Univ. (Portugal). Dept. de Quimica, and Imperial Coll. of Science and Technology, London (Eng-

Included in Jnl. of Physical and Chemical Reference Data, v19 n1 p113-116 1990. Available from American Chemical Society, 1155 16th St., NW, Washington, DC

Keywords: \*Benzene, \*Thermal conductivity, \*Standards, Liquids, Literature surveys.

The available experimental liquid-phase thermal conductivity data for benzene have been examined with the intention of establishing a further liquid thermal conductivity standard along the saturation line. The quality of the available data is such that new standard reference values can be proposed with confidence limits better than + or - 1% for most of the normal liquid range. (Copyright (c) 1990 by the U.S. Secretary of Commerce.)

100.256

PB90-244591

(Order as PB90-244526) R and D Associates, Marina del Rey, CA.

**Updated Excitation and Ionization Cross Sections** for Electron Impact on Atomic Oxygen.

Quarterly rept.
R. R. Laher, and F. R. Gilmore. c1990, 29p
Contract DNA-001-85-C-0022
Sponsored by Defense Nuclear Agency, Washington, DC.

Included in Jnl. of Physical and Chemical Reference Data, v19 n1 p277-304 1990. Available from American Chemical Society, 1155 16th St., NW, Washington, DC

Keywords: Upper atmosphere, Excitation, Tables(Data), Graphs(Charts), \*Electron-atom collisions, \*Oxygen atoms, lonization cross sections, Electron in the contraction of the contractio tron impact.

Cross sections for the excitation and ionization of atomic oxygen by electron impact are presented as the result of a critical review of experimental and theoreti-cal work on this subject. An effort has been made to compile the most accurate and complete set of cross sections available. More than 60 profiles of excitation cross section versus electron-impact energy are presented. These include transitions to the forbidden metastable O(2p(4) singlet D) and O((2p(4) singlet s) states, the allowed autoionizing O(2p(5) triplet p(0)) state, nine allowed Rydberg series, and twenty-nine forbidden Rydberg series. Recommended ionization cross sections for transitions to the various outer-electron ionization states to the inner-electron ionization state O(1+) quartet p, and to the O(2+) state are also given. The data presented in the report will be useful in calculations of aeronomical and artificially-induced electron impact on atomic oxygen, an important component of the upper atmosphere. (Copyright (c) 1990 by the U.S. Secretary of Commerce.)

100,257

PB90-244609 Not available NTIS American Chemical Society, Washington, DC.

Journal of Physical and Chemical Reference Data,

Volume 19, Number 2, 1990.

Volume 19, Number 2, 1990.

Quarterly rept.

D. R. Lide. c1990, 208p

See also PB90-244617 through PB90-244641 and

PB90-244526. Prepared in cooperation with American
Inst. of Physics, New York. Sponsored by National
Inst. of Standards and Technology, Gaithersburg, MD.

Available from American Chemical Society, 1155 16th St., NW, Washington, DC 20036.

Keywords: \*Physical chemistry, Thermodynamic properties, Chemical properties, Aromatic polycyclic hydro-carbons, Physical properties, Dielectric properties, Water, Reaction kinetics, Photochemical reactions, \*Reference materials, Debye-Huckel theory, Isomers, Peroxyl radicals, Aqueous solutions.

Contents: Standard Chemical Thermodynamic Properties of Isomer Groups of Monochloroalkanes; Standard Chemical Thermodynamic Properties of Polycyclic aru Chemicai Thermodynamic Properties of Polycyclic Aromatic Hydrocarbons and Their Isomer Groups. III. Naphthocoronene Series, Ovalene Series, and First Members of Some Higher Series; The Dielectric Constant of Water and Debye-Huckel Limiting Law Slopes; Rate Constants for Reactions of Peroxyl Radicals in Fluid Solutions; Cumulative Listing of Reprints and Supplements Supplements.

100.258 PB90-244617

(Order as PB90-244609) Massachusetts Inst. of Tech., Cambridge. Dept. of

Chemistry.

Standard Chemical Thermodynamic Properties of Isomer Groups of Monochloroalkanes.

Quarterly rept. R. A. Alberty, and M. B. Chung. c1990, 28p Sponsored by National Inst. of Standards and Tech-

nology, Gaithersburg, MD.
Included in Jnl. of Physical and Chemical Reference
Data, v19 n2 p321-348 1990. Available from American
Chemical Society, 1155 16th St., NW, Washington, DC

20036.

Keywords: \*Thermodynamic properties, \*Chloroal-kanes, Standards, Gibbs free energy, Enthalpy, Entro-py, Specific heat, Tables(Data), Chemical properties, Physical properties, Physical chemistry, \*Isomers, \*Reference materials, Benson method.

The chemical thermodynamic properties of isomer groups of monochloroalkanes from C2H5Cl to C8H17Cl in the ideal gas phase have been calculated

from 298.15 to 1500 K using new Benson group values from Bozzelli. Increments in isomer group properties per CH2 have been calculated to show the extent to which thermodynamic properties of higher isomer groups may be obtained by linear extrapolation. Equilibrium mole fractions within isomer groups have been calculated for the ideal gas state. Values of Cp, S, delta (sub f) H, and delta (sub g) G are given for all species of monochloroalkanes from CH3Cl to C8H17Cl in SI units for a standard state pressure of 1 bar. The values calculated here are compared with values published by the Thermodynamics Research Center (Texas A and M University) on June 30, 1981. (Copyright (c) 1990 by the U.S. Secretary of Commerce.)

PB90-244625

(Order as PB90-244609) Massachusetts Inst. of Tech., Cambridge. Dept. of

Chemistry.

Standard Chemical Thermodynamic Properties of Polycyclic Aromatic Hydrocarbons and Their Isomer Groups. III. Naphthocoronene Series, Ovalene Series, and First Members of Some Higher Series.

Quarterly rept R. A. Alberty, M. B. Chung, and A. K. Reif. c1990,

Sponsored by National Inst. of Standards and Tech-

nology, Gaithersburg, MD. Included in Jnl. of Physical and Chemical Reference Data, v19 n2 p 349-370 1990. Available from American Chemical Society, 1155 16th St., NW, Washington, DC

Keywords: \*Thermodynamic properties, \*Aromatic polycyclic hydrocarbons, Standards, Numerical analysis, Molecular structure, Gibbs free energy, Tables(Data), Enthalpy, Specific heat, Chemical properties, Naphthalene compounds, Entropy, Physical chemistry, \*Isoners, \*Reference materials, Benson method, Ovalenes.

The tables in the first two papers on polycyclic aromatic hydrocarbons (J. Phys. Chem. Ref. Data 17,241 (1988) and J. Phys. Chem. Ref. Data (18, 77 (1989)), have been extended by calculating thermodynamic properties for the first two isomer groups in the naphtherecords. ocoronene series, the first two isomer groups in the ovalene series, and first members of some higher series. Successive isomer groups in each series differ by C4H2. The properties of individual species have been estimated using Benson group values of Stein and Fahr for temperatures from 298.15 to 3000 K. Values of C(sub p), S, delta(sub f) H, and delta(sub f) G for a standard state pressure of 1 bar are given for isomer groups and for individual species. The isomer group values provide a basis for extrapolating to higher carbon numbers where it is not feasible to consider individual molecular species. (Copyright (c) 1990 by the U.S. Secretary of Commerce.)

100,260 PB90-244633

(Order as PB90-244609) National Inst. of Standards and Technology, Gaithers-

Dielectric Constant of Water and Debye-Huieckel Limiting Law Slopes.

Quarterly rept. D. G. Archer, and P. Wang. c1990, 41p Included in Jnl. of Physical and Chemical Reference Data, v19 n2 p371-412 1990. Available from American

Chemical Society, 1155 16th St., NW, Washington, DC Keywords: \*Dielectric properties, \*Water, Physical

Reywords: "Defectific properties, Water, Frigsteal properties, Thermodynamic properties, Graphs(Charts), Numerical analysis, Tables(Data), Equations of state, Physical chemistry, Comparison, Experimental design, Specific heat, Enthalpy, Osmosis, Volume, "Reference materials, "Debye-Huckel theory.

Experimental values of the dielectric constant of water suggest that, for temperatures greater than 400 K, the integral in the Kirkwood dielectric-constant equation, which involves the intermolecular potential function, is a simpler function of temperature and pressure than of temperature and density. An equation has been fitted to values of this integral calculated from experimental values of the dielectric constant for temperatures from 238.15 K to 823.15 K and to pressures of approximately 500 MPa for temperatures greater than 273 K. The equation for epsilon thus has explicit variables T, rho, p

and gives a good representation of the available experimental results. The quality of representation of the experimental results has been compared to that of previous correlations of the dielectric constant. The new equation is applicable through wider regions of independent variables than the previous equations and is capable of sufficient accuracy to provide values of Debye-Huckel limiting law slopes which are as accurate as the experimental results allow. Values of Debye-Huckel limiting-law slopes are tabulated. (Copyright (c) 1990 by the U.S. Secretary of Commerce.)

100,261 PB90-244641

(Order as PB90-244609)

Notre Dame Univ., IN. Radiation Lab.
Rate Constants for Reactions of Peroxyl Radicals in Fluid Solutions.

Quarterly rept.
P. Neta, R. E. Hue, and A. B. Ross. c1990, 161p
Sponsored by National Inst. of Standards and Technology (NML), Gaithersburg, MD. Chemical Kinetics

Included in Jnl. of Physical and Chemical Reference Data, v19 n2 p413-515 1990. Available from American Chemical Society, 1155 16th St., NW, Washington, DC 20036

Keywords: \*Reaction kinetics, Physical chemistry, Chemical reactions, Alkanes, Photolysis, Radiolysis, Chemical properties, Biochemistry, Photochemical reactions, Atmospheric chemistry, Tables(Data), Solvents, \*Peroxyl radicals, \*Aqueous solutions.

Absolute rate constants for reactions of alkylperoxyl and substituted alkylperoxyl radicals with inorganic and organic compounds in aqueous and non-aqueous fluid solutions have been compiled. The radicals have been generated by radiolysis or photolysis and their rate constants were determined generally by kinetic spectrophotometry or esr. Rate constants are included also for formation of peroxyl radicals by reaction of alkyl radicals with oxygen and for decay of peroxyl radicals by radical-radical reactions. (Copyright (c) 1990 by the U.S. Secretary of Commerce.)

100,262 PB90-244658 Not available NTIS American Chemical Society, Washington, DC.

Journal of Physical and Chemical Reference Data,
Volume 19, Number 3, 1990.

Quarterly rept.
D. R. Lide. c1990, 294p
See also PB90-244666 through PB90-244724 and PB90-244609. Prepared in cooperation with American Inst. of Physics, New York. Sponsored by National Inst. of Standards and Technology, Gaithersburg, MD. Available from American Chemical Society, 1155 16th St., NW, Washington, DC 20036.

Keywords: \*Research, Collision cross sections, Atomic energy levels, Water vapor, Steam, Specific heat, Alcohol, Carbon dioxide, Photon-atom collisions, Electron-atom collisions, Electron-molecule collisions, Electron-ion collisions, Hydrogen ions, Oxygen atoms, Copper ions, Atom-molecule collisions, Molecule-molecule collisions, Ion-molecule collisions, Refractive index, Alkyl alcohols.

Contents: Energy Levels of Copper, Cu I through Cu XXIX; Cross Sections and Related Data for Electron Collisions with Hydrogen Molecules and Molecular lons; Cross Sections for Collisions of Electrons and Photons with Atomic Oxygen; Cross Sections and Swarm Coefficients for H(1+), H2(+), H3(+), H, H2, and H(1-) in H2 for Energies from 0.1 eV to 10 keV; Refractive Index of Water and Steam as Function of Wavelength, Temperature and Density; Heat Capacities of Organic Compounds in the Liquid State I. C1 to C18 1-Alkanols; The Transport Properties of Carbon Dioxide.

100,263 PB90-244674

(Order as PB90-244658) National Inst. for Fusion Science, Nagoya (Japan).
Cross Sections and Related Data for Electron Collisions with Hydrogen Molecules and Molecular lons.

Quarterly rept. H. Tawara, Y. Itikawa, H. Nishimura, and M. Yoshino. c1990, 20p

Prepared in cooperation with Institute of Space and Astronautical Science, Sagamihara (Japan), Niigata Univ. (Japan). Dept. of Physics, and Shibaura Inst. of Tech., Tokyo (Japan).

Included in Jnl. of Physical and Chemical Reference Data, v19 n3 p617-635 1990. Available from American Chemical Society, 1155 16th St., NW, Washington, DC

Keywords: \*Collision cross sections, Excitation, Dissociation, Ionization, \*Electron-molecule collisions, \*Electron-ion collisions, \*Hydrogen ions, Molecular ions, Electron impact, Attachment, Rotational states, Vibrational states, Recombination.

Data are compiled and evaluated for collision processes of excitation, dissociation, ionization, attachment, and recombination of hydrogen molecules and molecular ions (H2(1+), H3(1+)) by electron impact as well as for properties of their collision products. (Copyright (c) 1990 by the U.S. Secretary of Commerce.)

100,264 PB90-244682

(Order as PB90-244658) Institute of Space and Astronautical Science, Sagamihara (Japan).

Cross Sections for Collisions of Electrons and Photons with Atomic Oxygen.

Quarterly rept.

Y. Itikawa, and A. Ichimura. c1990, 13p Included in Jnl. of Physical and Chemical Reference Data, v19 n3 p637-650 1990. Available from American Chemical Society, 1155 16th St., NW, Washington, DC

Keywords: \*Collision cross sections, Atomic energy levels, Scattering cross sections, Excitation, tron-atom collisions, \*Photon-atom collisions, Oxygen atoms, Photoionization, Oscillator strengths.

Data have been compiled on the cross sections for the collisions of electrons and photons with atomic oxygen The processes considered are total scattering, elastic scattering, momentum transfer, excitations of electronic states (including fine structure levels of the ground state), ionization, and electron attachment. The cross-section data are presented graphically. Energy levels, transition probabilities and some other properties of atomic oxygen are summarized to aid un-derstanding of the collision processes. The literature was surveyed through December 1988, but more recent data, if they are available to the authors, are included also. (Copyright (c) 1990 by the U.S. Secretary of Commerce.)

100,265 PB90-244716

(Order as PB90-244658) Vysoka Skola Chemicko-Technologicka, Prague (Czechoslovakia). Heat Capacities of Organic Compounds in the

Liquid State I. C1 to C18 1-Alkanols.

Quarterly rept. M. Zabransky, V. Ruzicka, and V. Majer. c1990, 44p Grant NBS-60NANB9DO912

Prepared in cooperation with Delaware Univ., Newark.

Dept. of Chemistry. Sponsored by National Inst. of Standards and Technology, Gaithersburg, MD. Included in Jnl. of Physical and Chemical Reference Data, v19 n3 p719-760 1990. Available from American Chemical Society, 1155

Keywords: \*Specific heat, \*Alcohols, Liquids, Polynomials, Tables(Data), Spline functions, Calorimetry, Temperature dependence, Methanol, Ethanol, Alkyl alcohols, Propanols, Butanols.

Heat capacities of liquid C1 to C18 1-alkanols measured by calorimetric methods were compiled and evaluated. The selected experimental data were fitted as a function of temperature with cubic splines using weighted least squares minimization. The parameters of the cubic spline polynomials and the recommended values for heat capacities are presented. A new quasipolynomial equation which permits extrapolation of heat capacities outside the temperature range of experimental values was derived and its parameters for C1 to C10 1-alkanols are presented. (Copyright (c) 1990 by the U.S. Secretary of Commerce.)

100.266 PB90-244724

(Order as PB90-244658) Imperial Coll. of Science and Technology, London (England). Dept. of Chemical Engineering and Chemical Technology.

# **Physical & Theoretical Chemistry**

Transport Properties of Carbon Dioxide.

Quarterly rept.
V. Vesovic, W. A. Wakeham, G. A. Olchowy, J. V. Sengers, J. T. R. Watson, and J. Millat. c1990, 46p
Prepared in cooperation with Maryland Univ., College
Park. Inst. for Physical Science and Technology, National Engineering Lab., East Kilbride (Scotland), and

Rostock Univ. (German D.R.). Included in Jnl. of Physical and Chemical Reference Data, v19 n3 p763-808 1990. Available from American Chemical Society, 1155 16th St., NW, Washington, DC

20036

Keywords: \*Carbon dioxide, \*Thermal conductivity, \*Viscosity, Thermodynamic properties, Transport properties.

The paper contains new, representative equations for the viscosity and thermal conductivity of carbon dioxide. The equations are based in part upon a body of experimental data that have been critically assessed for internal consistency and for agreement with theory whenever possible. In the case of the low-density ther mal conductivity at high temperatures, all available data are shown to be inconsistent with theoretical expectation and have therefore been abandoned in favor of a theoretical prediction. Similarly, the liquid-phase thermal conductivity has been predicted owing to the small extent and poor quality of the experimental information. The complete correlations cover the temperature range 200 K = or < T < 1500 K for viscosity and 200 K = or < T = or < 1000 K for thermal conductivity, and pressures up to 100 MPa. Tables of the viscosity and the viscosity and pressures up to 100 MPa. Tables of the viscosity and pressures up to 100 MPa. ty and thermal conductivity generated by the repre-sentative equations are provided to assist with the confirmation of computer implementations of the calculation procedure.

PB91-134494 Not available NTIS

Not available NTIS
National Inst. of Standards and Technology (NML),
Boulder, CO. Thermophysics Div.
Critical Locus, (Vapor + Liquid) Equilibria, and Coexisting Densities of (Carbon Dioxide + Propane)
at Temperatures from 311 K to 361 K.

Final rept.
V. G. Niesen, and J. C. Rainwater. 1990, 19p
Sponsored by Department of Energy, Washington, DC. Office of Basic Energy Sciences.

Pub. in Jnl. of Chemical Thermodynamics 22, p777-795 1990.

Keywords: \*Thermodynamic equilibrium, \*Carbon dioxide, \*Propane, Measurement, Vapors, Liquids, Density(Mass/volume), Critical point, Critical pressure, Correlation, Comparison, Mathematical models, Dew point, Wet bulb temperature, Reprints, Temperature dependence.

Isothermal (vapor + liquid) equilibria and coexisting densities for (carbon dioxide + propane) have been measured at (311.05, 327.75, 344.43, and 361.15) K from the vapor pressure of propane to the critical pressure of the mixture, and the critical locus has thus been determined. Away from the critical locus, the measurements agree within combined experimental uncertainties with those of Reamer, Sage, and Lacey. The measurements confirm the observation of Roof and Baron that the critical pressures reported by Poettmann and Katz and by Reamer et al. are substantially in error. The critical pressures from the study are lower than those of Reamer et al. by as much as 0.785 MPa and of Roof and Baron by as much as 0.034 MPa. The and of Hoof and Baron by as much as 0.034 MPa. The dew- and bubble-points are correlated by three methods, the Soave-Redlich-Kwong (SRK) equation, the DDMIX program of Ely, and the Leung Griffiths model as modified by Moldover and Rainwater. Except for poor predictions of liquid densities by the SRK equation, all three models provide good correlations of the measurements, but the modified Leung-Griffiths model is superior very near the critical locus.

Not available NTIS PB91-134676 National Inst. of Standards and Technology (NML), Boulder, CO. Thermophysics Div.

Neutron Diffraction from Sheared D-Glycerol: Pre-

liminary Studies.

G. C. Straty, and H. J. M. Hanley. 1988, 8p Sponsored by Department of Energy, Washington, DC.

Office of Basic Energy Sciences.
Pub. in Proceedings of Symposium on Energy Engineering Sciences (6th), May 4-6, 1988, p136-143.

Keywords: Neutron diffraction, Supercooling, Shear properties, Reprints, \*Glycerols, Structure factors.

The paper reports on the experimental segment of a wide range investigation of the nature of complexity in liquids, as manifested by their behavior under mechanical stress. An apparatus constructed for a feasibility study of such behavior is described. Preliminary neutron diffraction measurements of the static structure factor of supercooled liquid glycerol under shear are reported. Data were taken on the SANS facility at NBS in the range 0.02 = or < Q = or < 0.39/A, Q equal to 0.8, 1.35, and 3.5/A. Comparisons between the sheared data and data for the system at equilibrium are given. The tentative conclusion is that the influof shear on the structure factor may be strong, but the data are too qualitative for a significant interpretation.

100,269 PB91-134957 Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Thermophysics Div. Structure of a Stage-3 Cs - Graphite Intercalate.

P. A. Wielopolski, J. W. White, and H. J. M. Hanley. 1990, 11p Pub. in Molecular Physics 69, n6 p947-957 1990.

Keywords: \*Graphite, \*Cesium, Computerized simulation, Structural analysis, Reprints, \*Intercalation, Molecular dynamics, Temperature dependence, Multilavers.

The influence of interlayer coupling on the in-plane structural properties of the stage-3 cesium-graphite system is investigated using a multilayer molecular-dynamics simulation. It is shown that the in-plane structure, represented by the circularly averaged pair distribution function, is insensitive to the interlayer coupling over a wide range of temperatures. The structure of the layer is investigated as a function of the parameters of the Cs-Cs potential and of the barrier height for free diffusion created by the graphite periodic po-

PB91-146985 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.

Adsorption of Water and Oxygen on Ag(110): A Study of the Interactions among Water Molecules, Hydroxyl Groups, and Oxygen Atoms. Final rept.

K. Bange, T. E. Madey, J. K. Sass, and E. M. Stuve. 1987, 29p Pub. in Surface Science 183, n3 p334-362 1987.

Keywords: \*Water, \*Oxygen, \*Chemisorption, \*Surface chemistry, Silver, Electron beams, Desorption, Chemical bonds, Hydroxyl radicals.

The adsorption of water on clean and oxygen covered Ag(110) in ultra-high vacuum was studied with thermal desorption spectroscopy (TDS), electron stimulated desorption ion angular distribution (ESDIAD), low energy electron diffraction (LEED), work function measurements, and Auger electron spectroscopy. Water adsorbs on the clean surface at 80 K with no long-range order and only weak short-range order as determined by LEED and ESDIAD, respectively. Electron bombardment of water adlayers on clean Ag(110) results in dissociation to form OH groups at 80 K. Water also reacts with preadsorbed oxygen, either in atomic or molecular form, to form OH groups at 80 K. The O-H bond axis of the OH groups is tilted with respect to the surface normal and its thermodynamically stable, azimuthal orientation is along the (001) direct tion. In the absence of excess, molecular H2O, the OH groups exhibit no hydrogen bonding. The OH groups form (lxm) (m = 2,3) LEED compression patterns upon annealing to 200 K. These LEED patterns require the OH groups to diffuse across the ridges of the surface. The gamma adsorption state, which evolves water in a desorption peak at 225 K, was carefully studied. This state consists of coadsorbed H2O and OH in a 1:2 ratio. The results of the work are combined with earlier TDS and vibrational measurements for this system to propose an adsorption model for the gamma state, in which the H2O molecules are hydrogen bonded to the OH groups and the OH groups occupy a binding site different from the case where no excess water exists.

100 271

Not available NTIS PB91-147009 National Inst. of Standards and Technology (NML), Gaithersburg, MD. Thermophysics Div.

Critical Exponent for Viscosity.

Final rept.

R. F. Berg, and M. R. Moldover. 1990, 4p Sponsored by National Aeronautics and Space Administration, Washington, DC.
Pub. in Physical Review A 42, n12 p7183-7186, 15 Dec

Keywords: \*Viscosity, \*Carbon dioxide, \*Xenon, Liquefied gases, Critical point, Reduced gravity, Exponents, Reprints.

The authors have measured the critical exponent y characterizing the divergence of the viscosity eta varies as absolute value of (T-T(c))(sup(-y)) for carbon dioxide and xenon. The values of y for both fluids fall within the range y=0.041 + or - 0.001 and are conwithin the range y=0.041 + or - 0.001 and are consistent with the range y=0.042 + or - 0.002 spanned by the earlier data for four binary liquid mixtures. The agreement is the strongest evidence that pure fluids and binary liquids are in the same dynamic universality class; however, the results for y are inconsistent with the recent theoretical value of 0.032.

100.272

PB91-147041 Not available NTIS Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Chemical Engineering Science Div. Heat Capacity and Thermodynamic Properties of Deuterated Ammonium Hexafluorophosphate ND4PF6 from 5.8 K to 347 K.

Final rept.

J. E. Callanan, R. D. Weir, and E. F. Westrum. 1990, 12p

Sponsored by Department of National Defence, Ottawa (Ontario). Pub. in Jnl. of Chemical Thermodynamics 22, p979-990 1990.

Keywords: \*Specific heat, \*Calorimetry, \*Ammonium compounds, \*Inorganic phosphates, Isotopic labeling, Temperature dependence, Thermodynamic properties, Deuteration, Tables(Data), Order disorder transformations, Reprints.

The heat capacity of deuterated ammonium hexafluor-ophosphate ND4PF6 was measured from 5.8 K to 347 K by adiabatic calorimetry. Two lambda-shaped anomalies were found in the curve for heat capacity against temperature. The upper anomaly reached a peak heat capacity (at constant pressure) of approx 600R at (194.4 + or - 0.05) K with Delta(sub trs)S(sup 0) = (1.013 + or - 0.016) R(R = 8.3145 J/K/mol). The lower anomaly is also lambda-shaped but is gradual, continuous, and reaches its maximum heat capacity = 19.2 R at (137.5 + or - 1.0)K with Delta(sub trs)S(sup 0) = (0.562 + or - 0.011) R. Both anomalies are characteristic of order-disorder transitions. Smoothed values of the standard thermodynamic quantities are tabulated up to 350 K.

100.273

PR91-147058 Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Chemical Engineering Science Div. Heat Capacity of Deuterated Ammonium Tetra-fluoroborate ND4BF4 from 7 to 348 K.

Final rept. J. E. Callanan, R. D. Weir, and E. F. Westrum. 1990,

12p Sponsored by Department of National Defence, Ottawa (Ontario). Pub. in Jnl. of Chemical Thermodynamics 22, p957-

968 1990.

Keywords: \*Calorimetry, \*Ammonium compounds, \*Fluoborates, \*Specific heat, Isotopic labeling, Deuteration, Temperature dependence, Tables(Data), Thermodynamic properties, Order disorder transformations, Reprints, \*Foreign technology.

The heat capacity of deuterated ammonium tetrafluoroborate ND4BF4 was measured at constant pressure from 7 K to 348 K by adiabatic calorimetry. The curve for heat capacity against temperature is smooth with a broad maximum between 120 K and 165 K, and the peak value of approximately 14.9 R occurs between 145 K to 155 K. The shape of the broad maximum is similar to that found in other anisotropic salts and is believed to be a result of contributions both from the rotation of the ND4(sup +) ion and from a larger than usual dilation of the unit cell. Values of the standard thermodynamic quantities are tabulated up to 350 K.

100,274

PR91-147157 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Organic Analytical Research Div.

Cryogenic-Temperature Fluorescence Spectra of Polynuclear Aromatic Hydrocarbons of Molecular Weight 302. Final rept.

A. L. Colmsjo, and S. A. Wise. 1986, 9p Pub. in Analytica Chimica Acta 187, p129-137 1986.

Keywords: \*Aromatic polycyclic hydrocarbons, \*Fluorescence spectroscopy, \*Pyrenes, Cryogenics, Sensitivity, Selectivity, Molecular weight, Reprints, \*Fluoranthenes, \*Perylenes, \*Shpol'skii effect.

Shpol'skii cryogenic temperature fluorescence spectra of 19 of the possible 33 polynuclear aromatic hydrocarbons with a molecular weight of 302 are reported. The group consists of the benzo- and naphtho-pyrenes and fluoranthenes and also the benzoperylenes. There is a large variation in the degree of selectivity and sensitivity achieved by the Shpol'skii technique within this group of compounds.

100.275

PB91-147199 Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Chemical Engineering Science Div. Hydrogen Slush Production with a Large Auger. Final rept.

D. E. Daney, V. D. Arp, and R. O. Voth. 1990, 10p Sponsored by National Aeronautics and Space Admin-istration, Cleveland, OH. Lewis Research Center. Pub. in Advances in Cryogenic Engineering 35, p1767-1776 1990.

Keywords: \*Cryogenics, \*Solid cryogens, \*Solidified gases, \*Augers, Refrigerants, Mathematical models, Generators, Slush, Reprints, \*Solid hydrogen.

The design and construction of a 178 mm (7 in) diamere auger type hydrogen slush generator is described. A supercritical helium flow loop, which simulates the performance of a helium refrigerator, cools the generator. The coolant temperature varies down to 5 K and the flow varies about the 1.4 L/s (3 cfm) design point. The computer model of the auger type generator shows that coolant temperature and auger speed have the greatest influence on slush production rate, although coolant flow rate and auger radial clearance are also important. All these effects will be evaluated in the tests of the system.

100,276 PB91-147298 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.

Soluble Models in Surface Collision Dynamics. Final rept.

J. W. Gadzuk. 1988, 7p

Pub. in Solvay Conference on Surface Science, v14 p310-316 1988.

Keywords: \*Molecular collisions, \*Surface reactions, Molecular excitation, Dynamics, Phonons, Reprints.

Aspects of electron-hole pair, phonon, and intra-mo-lecular vibrational excitation, as illustrated in some soluble models in surface collision dynamics, are considered. Emphasis is placed on energy redistribution and sticking out metal surfaces.

PB91-147363 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Thermophysics Div. Limiting versus Apparant Critical Behavior of Henry's Constants and K Factors.

Final rept. A. H. Harvey, R. Crovetto, and J. M. H. Levelt Sengers. 1990, 4p

Pub. in AIChE Jnl. 36, n12 p1901-1904 Dec 90.

Keywords: Asymptotic properties, Critical point, Thermodynamics, Solubility, Mixtures, Reprints, \*Henry

In previous work, an asymptotic relationship, linear with the appropriate choice of variables, was derived for the variation of Henry's constant for a solute in the neighborhood of the solvent's critical point. When experimental Henry's-constant data in several solvents were plotted in a manner suggested by the asymptotic relationship, linearity was observed over a wide range

of conditions. Since these lines remained straight at the highest (closet-to-critical) temperatures at which data existed, it was assumed that they represented the asymptotic behavior. Further study, however, has shown that this assumption is mistaken and that the Henry's-constant plot attains its asymptotic behavior only in a small region closer to the critical point than the extent of the data. A related asymptotic linear relationship involving the vapor-liquid partition coefficient (K-factor) appears to be a more reliable indicator of the true asymptotic behavior, in part because the limiting value at the critical point is known a priori. The work explains the discrepancy noted in previous work be-tween slopes of Henry's-constant plots and the initial slopes of mixture critical lines.

100,278 PB91-147405

Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Thermophysics Div.

Extension of an Improved One-Fluid Conformal Solution Theory to Real Fluid Mixtures with Large Size Differences.

Final rept.

M. L. Huber, and J. F. Ely. 1990, 10p Sponsored by Department of Energy, Washington, DC. Pub. in International Jnl. of Thermophysics 11, n1 p87-96 Jan 90.

Keywords: \*Fluids, Lennard-Jones potential, Perturbation theory, Statistical mechanics, Helmholtz free energy, Hydrocarbons, Mixtures, Reprints.

Conformal solution theories have been shown to be inadequate as the size ratio of the molecules in a mixture increases. The authors present an improved van der Waals-1 fluid conformal solution theory which incorporates a correction term developed using statistical mechanical perturbation theory. The correction addresses the effect of different size molecules on the Helmholtz free energy of the mixture. Results of the new model are compared with other conformal solution theories for model Lennard-Jones systems. They also show how to extend the model to perform computations on real fluid mixtures. Results for selected hydrocarbon mixtures are given.

100,279 PB91-147454 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Molecular Spectroscopy Div.

Structure of Carbon Dioxide Dimer from Near Infrared Spectroscopy.

Final rept.

K. W. Jucks, Z. S. Huang, D. Dayton, R. E. Miller, and W. J. Lafferty. 1987, 6p Pub. in Jnl. Chemical Physics 86, n8 p4341-4346 1987.

Keywords: \*Molecular structure, Near infrared radiation, Infrared spectra, Dimers, Reprints, \*Carbon dioxide dimers.

An F-center laser-molecular beam spectrometer has been used to obtain a sub-Doppler resolution spectrum of the CO2 dimer. The vibrational mode investigated in corresponds to the nu(1) + nu(3) combination band of the monomer located at 3716/cm. A qualitative assignment of the spectrum shows that the equilibrium structure of the molecule has C(2h) symmetry, as, due to zero spin nuclei, half of the expected transitions are missing in the observed spectrum. This implies that the molecule has a slipped parallel structure rather than a T-shaped geometry.

PB91-147470 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Chemical Kinetics Div.

Alkyl Transfer Reactions between Protonated Alcohols and Ethers. The Gas-Phase Alkylation of Formaldehyde.

Final rept.

Z. Karpas, and M. Mautner. 1989, 5p Pub. in Jnl. of Physical Chemistry 93, n5 p1859-1863

Keywords: \*Organic ions, \*Alcohols, \*Ethers, \*Reaction kinetics, Stability, Chemical reactivity, Activation energy, Molecular structure, Reprints, \*Alkyl transfer reactions.

Alkyl transfer reactions between protonated ethers and alcohols are of the general type R2OR(prime)(+) + R(double prime)2O ---> R(double prime)2OR(prime)(+) + R2O, where R = H or an alkyl radical. The reactions are classified according to

the degree of alkylation, with up to n=5 alkyl groups in the system. For n=2 the reaction is alkyl transfer between alcohols ROH2(+) and ROH to yield protonated ethers R2OH(+). The rate constants for these reactions increase with increasing stability of the transferred R(+) group, possibly due to lowered activation ferred H(+) group, possibly due to lowered activation barrier of the initial partial R(+)-OH2 dissociation. However, the reaction with R(+)=CH3(+) is faster and with R(+)=1-C4H9(+) is slower than expected, possibly due to steric effects. For n=3, i.e., reactions between the ethers R2OH(+) and the alcohols R(prime)OH, both the formation of R(prime)ORH(+) and of the tertiary oxonium ions R2OR(prime)(+) are observed. For n = 4, the reaction between the ethers R2OH(+) and R2O to give R2OR(+) is observed. For n = 5, a completely alkylated system, an example is methyl exchange between (CH3)2OCD3(+) and (CH3)2O, which is a very slow thermoneutral reaction with a large activation energy of 13 kcal/mol.

100.281

PB91-147538 Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Chemical Process Metrology Div. Instability in pH Measurements of Sputtered IrO2

Films.

K. G. Kreider, S. Semancik, and J. E. Erickson. 1987, 4p

Pub. in Proceedings of International Conference on Sensors and Actuators (4th) - Transducers '87, Tokyo, Japan, June 2-5, 1987, p734-737.

Keywords: \*Iridium oxides, \*pH meters, pH value, Instability, Sensors, Thin films, Photoelectron spectroscopy, Crystallinity, Amorphous materials, Reprints.

Sputter deposition of iridium oxide can produce thin films that show significant promise for use as the active coating in pH sensing devices. Among the desirable characteristics of sputtered iridium oxide films are their superior corrosion resistance, high temperature capabilities, and their ability to be fabricated in forms suitable for miniaturized probes. The results of testing of SIROF pH sensors produced in the study indicate that both anhydrous, crystalline films and amorphous films yield similar responses of approximately 56-59 mv/pH. The open circuit potential of these films did vary with various fabrication conditions and environmental exposures. Deliberate attempts to modify the open circuit potential of the SIROFs included air baking at 523K, which significantly increased the output voltage and autoclave heating at 523K, which significantly decreased the voltage. XPS measurements on SIROF films showed that iridium is present in a +4 oxidation for a variety of treatments. Oxygen in core level data suggest that certain test treatments considered here may cause surface hydroxylation.

100.282

Not available NTIS PB91-147645 National Bureau of Standards (NML), Gaithersburg, MD. Chemical Kinetics Div.

Resonance Enhanced Multiphoton Ionization

Spectroscopy of CHCI2 and CDCI2.

G. R. Long, and J. W. Hudgens. 1987, 3p Pub. in Jnl. of Physical Chemistry 91, p5870-5872 1987.

Keywords: Deuterium compounds, Rydberg states, Multi-photon processes, Ultraviolet spectra, Vibrational states, Reprints, \*Dichloromethane radicals, Multiphoton ionization.

Resonance enhanced multiphoton ionization spectra between 355 and 375 nm of CHCl2 and CDCl2 radicals are reported. The origin of the observed spectra was at 370.1 nm for CHCl2 and 370.4 nm for CDCl2. The REMPI mechanism is determined to be a 2 + 1 photon absorption, with the resonant intermediate state tentatively assigned as a 3d Rydberg state. Vibrational structure originated from activity in the C-Cl symmetric stretching and the out-of-plane bending modes. The C-CI symmetric stretch frequencies are 845/cm in CHCl2 and 814/cm in CDCI2.

100.283

PB91-147710 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Chemical Kinetics Div.

# **Physical & Theoretical Chemistry**

Multicomponent Cluster Ions. 2. Comparative Sta-bilities of Cationic and Anionic Hydrogen Bonded Networks: Mixed Clusters of Water and Hydrogen Cyanide. Final rept.

M. Mautner, and C. V. Speller. 1989, 4p.

See also AD-A167 880.
Pub. in Jnl. of Physical Chemistry 93, n9 p3663-3666

Keywords: \*Protons, \*Hydroxyl radicals, Hydration, Enthalpy, Acidity, Alkalinity, Stability, Hydrogen bonds, Reprints, \*Cyanide ions, \*Clusterions.

The thermochemistry of cluster ions containing H2O and HCN was obtained from clustering equilibria. The clustering of H2O about H3O(+) and OH(-), and the clustering of HCN about HCNH(+) show distinct shell filling effects, but the clustering of H2O and HCN about CN(-) does not. Hydration by one water molecule eliminates the difference of 5 kcal/mol between the proton affinities of HCN and H2O. Hydration also decreases the difference between the intrinsic deprotonation energies, ie., delta H(0) acid' of H2O and HCN from 37.7 kcal/mol, to 19.8 kcal/mol in the 4-fold hydrated species. In the protonated clusters, exchange of H2O by HCN does not significantly affect the total stability of the cluster.

PB91-147785 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Chemical Kinetics Div. Slow Electron Transfer Reactions between Alkyl-

hydrazines. Final rept.

S. F. Nelsen, D. T. Rumack, and M. Mautner. 1987,

Pub. in Jnl. of American Chemical Society 109, n5 p1373-1379 1987.

Keywords: \*Hydrazines, \*Reaction kinetics, \*Electron transfer, Organic ions, Gibbs free energy, Reprints, Energy barriers.

Unlike other gas-phase exoergic electron transfer reactions, reactions between alkylhydrazines, which involve large geometry changes, proceed with unusually low efficiencies, i.e., k/k(collision) = 0.01 - 0.0001. The temperature coefficient of Me2NNMe2 + Et-MeNNMeEt ---> EtMeNNMeEt(+) + Me2NNMe2. E(sub a) = +2.7 kcal/mol indicates an energy barrier of 16 kcal/mol for electron transfer within the complex. The energy barrier results from the large geometry change required for relaxation of the product R2NNR2(+) ions from a perpendicular to a planar geometry. Nevertheless, the energy barrier is substantially smaller than would result from vertical electron transfer in the complex (44 kcal/mol), indicating geometry. etry relaxation in the transition state. The major trends observed include: slowing of reactions of acyclic vs. cyclic reactants; and small positive or negative temperature coefficients. In these trends, electron transfer is similar to heavy particle transfer.

100.285 PB91-147801 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Chemical Kinetics Div.

Pulse Radiolysis Studies of Organic Electron

Transfer Reactions.

Final rept.

P. Neta, and A. Harriman. 1988, 53p

Pub. in Photoinduced Electron Transfer, Chapter 2.3, p110-162 1988.

Keywords: \*Porphyrins, \*Electron transfer, Oxidation reduction reactions, Organic ions, Radiolysis, Catalysts, Reprints.

Pulse radiolysis studies on organic electron transfer reactions are reviewed, with special emphasis on porphyrins and redox catalysts.

100,286 PB91-147884 Not available NTIS National Bureau of Standards (IMSE), Gaithersburg,

MD. Ceramics Div.

Effects of Pressure on the Thermal Decomposition Kinetics and Chemical Reactivity of Nitromethane. Final rept.

G. J. Piermarini, S. Block, and P. J. Miller. 1989, 6p Pub. in Jnl. of Physical Chemistry 93, n1 p457-462 1989

Keywords: \*Nitromethane, \*High pressure, \*Thermal degradation, \*Reaction kinetics, Chemical reactivity,

Isotope effect, Melting points, Ammonium formate, Water, Reprints

The effects of pressure and temperature on the melting point, thermal decomposition rate, and chemical reactivity of nitromethane have been studied. A diamond anvil high pressure cell in conunction with (1) an optical polarizing microscope for melting point and chemical reactivity observations, and (2) an automated Fourier transform infrared instrument for thermal decomposition kinetic measurements, were used. Both pressure and temperature were found to increase the rate of thermal decomposition indicating an overall bi-molecular reaction mechanism. However, the mechanism is complex and appears to vary over large changes in pressure. Nevertheless, a chemical mechanism is proposed which explains the bimolecularity and also accounts for the observed decomposition products, ammonium formate and water. A dynamic stress-induced catastrophic reaction in nitromethane, which appears to be crystal orientation dependent with respect to the applied stress, was found. Under the same conditions, deuterated nitromethane did not exhibit this catastrophic reaction.

100.287

Not available NTIS
National Inst. of Standards and Technology (NML),
Gaithersburg, MD. Surface Science Div.
Resonant Photoemics of the National Photoemics o Resonant Photoemission and PSD of Rare Earth

Oxides. Final rept

J. Schmidt-May, F. Senf, J. Voss, C. Kunz, and A. Flodstrom, 1985, 4p

Pub. in Desorption Induced by Electronic Transitions, DIET II, Springer Series in Surface Sciences, v4 p94-97 1985.

Keywords: \*Europium oxides, \*Samarium oxides, \*Ytterbium oxides, \*Photoemission, Photoelectron spectroscopy, Reprints, Photon stimulated desorption.

The resonant enhancement in photoelectron spectra at the 4d edges of rare earth atoms and metals is also found in photoyield spectra of desorbed ions from the surfaces of the oxides of Sm, Eu and Yb following the photon excitation. The analysis of the 4d 4f resonance leads to a picture of an indirect mechanism of ion desorption which is caused by the flux of energetic 4f bulk photoelectrons. Photoemission and ion desorption measurements of Sm metal with oxidized Yb overlayer strongly support this idea. The dominant desorption through secondary processes limits the use of the photon-stimulated desorption (PSD) in the sense that it is not known to which type of atom the desorbing species was attached.

100.288

PB91-148080 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Molecular Spectroscopy Div.

Fluoromethanol: Synthesis, Microwave Spectrum, and Dipole Moment. Final rept.

R. D. Suenram, F. J. Lovas, and H. M. Pickett. 1986,

Pub. in Jnl. of Molecular Spectroscopy 119, n2 p446-

Keywords: \*Carbinols, \*Fluorine organic compounds, \*Microwave spectra, \*Dipole moments, Synthesis(Chemistry), Rotational spectra, Electric moments, Conformational changes.

The microwave spectrum of the new molecular species CH2FOH has been observed and analyzed. The molecule exhibits a gauche conformation which is in accord with previous ab initio calculations. This is also the conformation that is predicted based on anomeric effect arguments. The rotational transitions are split by the tunneling of the molecule between equivalent gauche conformations. A simultaneous fit of both tunneling states allows the determination of perturbation free rotational parameters as well as the tunneling frequency and a tunneling distortion parameter. A dipole moment (dm) analysis yields values of all three dipole moment components and the dm(b)xdm(c) term which indicates that dm(b) and dm(c) have opposite signs.

100,289

PB91-148171 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Thermophysics Div. **Ergodic Convergence Properties of Supercooled** Liquids and Glasses.

Final rept.

D. Thirumalai, and R. D. Mountain. 1990, 14p See also PB90-254814. Sponsored by National Sci-

ence Foundation, Washington, DC. Pub. in Physical Review A 42, n8 p4574-4587, 15 Oct

Keywords: \*Supercooling, Amorphous materials, Ergodic processes, Binary alloys, Glass, Convergence, Reprints, Molecular dynamics.

The dynamical properties of two measures to probe ergodic behavior in Hamiltonian systems with a large number of degrees of freedom are investigated. The measures, namely, the energy metric d(t) and the fluctuation metric Omega(t) are both based on the timeaveraged energies of the individual particles compris-ing the system. These ideas are used to study the behavior of supercooled and glassy states of soft-sphere binary alloys using microcanonical molecular dynam-

100.290

PB91-148650 Not available NTIS National Inst. of Standards and Technology (NML),

Gaithersburg, MD. Molecular Physics Div.
Microwave Spectrum of Ar-H2O: Dipole Moment,
Isotopic Studies, and (17)O Quadrupole Coupling Constants.

Final rept. G. T. Fraser, F. J. Lovas, R. D. Suenram, and K. Matsumura. 1990, 16p

Pub. in Jnl. of Molecular Spectroscopy 144, p97-112

Keywords: \*Argon complexes, Microwave spectra, Deuterium compounds, Isotope effects, Oxygen 17, Oxygen 18, Dipole moments, Intermolecular forces, Van der Waals forces, Dimers, Water, Reprints.

Microwave spectra for the K = 0 states of Ar-H2O, Ar-D2O, Ar-HOD, Ar-H2(18)O, and Ar-H2(17)O were obtained using a pulsed-nozzle Fourier-transform microwave spectrometer. For the Ar-H2O species, the results are in excellent agreement with the far-infrared data of Cohen et al. (J. Chem. Phys. 89, 4494-4504 (1988) and 92, 169-177 (1990)). The present data are also compared with predictions from the three anisotropic potentials proposed by Hutson (J. Chem. Phys. 92, 157-168 (1990)) to interpret the far-infrared spectrum of the complex.

100,291

PB91-148726 Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Quantum Physics Div.

Photodissociation Dynamics of Water in the Second Absorption Band: Vibrational Excitation of OH (A (2)Sigma).

B. Heumann, K. Kuhl, K. Weide, R. Duren, B. Hess, U. Meier, S. D. Peyerimhoff, and R. Schinke. 1990,

Pub. in Chemical Physics Letters 166, n4 p385-390, 2 Mar 90.

Keywords: \*Water, \*Photodissociation, Excited states, Potential energy, Vibrational states, Excitation, Re-

A three-dimensional potential energy surface for the second excited state of water is caluclated by thsecond absorption band. The authors find, in accordance with experimental data, vibrational excitation of OH((Sup 2) Sigma) to be generally weak. This result can be readily explained in terms of the calculated potential surface.

100,292

PB91-148783 Not available NTIS National Inst. of Standards and Technology (NEL), Boulder, CO. Chemical Engineering Science Div. Kinetics of Copper Extraction Using (anti)-2-Hydroxy-5-Nonlybenzophenone Oxime.

Final rept. M. F. Jin, F. C. Michel, and R. D. Noble. 1989, 6p Pub. in Industrial and Engineering Chemistry Research 28, n2 p193-198 Feb 89.

Keywords: \*Copper complexes, \*Chelating agents, \*Oximes, \*Reaction kinetics, Transport properties, Liquid-liquid interfaces, Benzophenone, Decanes, Rotation Diffusion Position tation, Diffusion, Reprints.

For the reaction (Cu(2+)) (aq) + 2(HR)(org) (CuR2)(org) + 2(H(1+))(aq) using the chelating agent anti-2-hydroxy-5-nonylbenzophenone oxime, the reaction orders for (Cu++), the active isomer of the oxime, and (H+) were measured experimentally using a rotating diffusion cell. The reaction orders were first order in (Cu++), first order in the active isomer of oxime, and negative first order in (H+). Extrapolation of the diffusion cell data for the kinetically limited case was an important advancement of the technique. The forward and reverse reaction rate constants were calculated. The results were obtained using a resistance model of copper transport.

100,293 PB91-148841 Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Quantum Physics Div.

Mode Specific Internal and Direct Rotational Predissociation in HeHF, HeDF, and HeHCL: van der Waals Complexes in the Weak Binding Limit.

Final rept. C. M. Lovejoy, and D. J. Nesbitt. 1990, 21p Grant NSF-CHE86-05970

Sponsored by National Science Foundation, Washington, DC.

Pub. in Jnl. of Chemical Physics 93, n8 p5387-5407, 15 Oct 90

Keywords: \*Helium complexes, Hydrogen chloride, Hydrogen fluoride, Deuterium compounds, Van der Waals forces, Intermolecular forces, Infrared spectra, Predissociation, Reprints, Feshbach resonances, Supersonic expansion.

The near-infrared vibration-rotation spectra of the weakly bound complexes HeHF, HeDF, and HeHCl are observed in a slit supersonic expansion. The spectra correspond to simultaneous excitation of vibration and internal rotation of the H(D)X subunit within the complex. The HeHF and HeDF P/R branch transitions show J-dependent excess linewidths, which are attributed to rapid predissociation of the excited states from intramolecular rotation-translation energy transfer. The corresponding P/R branch transitions in HeHCl are not observed despite good S/N on the Q branch, suggesting even more rapid predissociation for the upper state of the complex. In addition to isotropic intermolecular potentials, the HeHF/HeDF data yield considerable information on the potential anisotropy in the region sampled by the bound and quasibound states. The information so obtained is complementary to results from scattering studies and provides sensitive tests for refining trial potential energy surfaces.

100,294 PB91-148882 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Molecular Physics Div. Structures of the NH3-HCCCCH and H2O-HCCCCH Complexes by Fourier-Transform Microwave Spectroscopy. Final rept.

K. Matsumura, F. J. Lovas, and R. D. Suenram. 1**99**0, 16p

Pub. in Jnl. of Molecular Spectrscopy 144, p123-138 1990.

Keywords: \*Complexes, \*Molecular structure, Acetylene, Ammonia, Water, Microwave spectra, Hydrogen bonds, Rotational spectra, Electric dipole moments, Dimers, Reprints, \*Ammonia complexes, \*Water com-plexes, Diacetylene, Fourier transform microwave spectroscopy.

The microwave spectra of the ammonia-diacetylene and water-diacetylene complexes have been observed with a pulsed-beam, Fabry-Perot cavity, Fourier-transform microwave spectrometer. In addition to the normal isotopic forms, the authors have also observed the spectra of ND3-HCCCCH, (15)NH3-HCCCCH, HDO-HCCCCH, and D2O-HCCCCH. Present results derived for the diacetylene complexes are compared with those of the acetylene complexes. It is noteworthy that the induced dipole moment of the ammonia-diacetylene complex is about 50% larger than that of the ammonia-acetylene complex. The effects of the conjugation of the carbon-carbon triple bonds are discussed.

100,295

PB91-148924 Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Quantum Physics Div.

Multireference-Configuration Interaction (MR-CI) Calculations on HS(2+) and Experimental Observation via Electron Impact Ionization of H2S

Final rept. P. J. Miller, S. A. Rogers, J. Senekowitsch, S. V. ONeil, and S. R. Leone. 1990, 15p Contract AFOSR89-0073

Sponsored by Air Force Office of Scientific Research, Bolling AFB, Washington, DC.
Pub. in International Jnl. of Mass Spectrometry and Ion

Processes 100, p505-519 1990.

Keywords: \*Hydrogen sulfides, Metastable state, Electron impact, Sulfur ions, Ionization, Reprints, Dictation.

The stability of the HS(2+) dictation is investigated both theoretically and experimentally. The theoretical analysis involves complete active-space self-consistent field (CASSCF) and multi-configuration reference-configuration interaction (MR-CI) theory. A metastable (sup 2)Pi ground state is found with a calculated barrier to dissociation of 1.52eV. No other metastable states for energies up to 10eV above the ground state are found. In conjunction with the theoretical results, electron impact ionization of H2S is able to generate the HS(2+) dication, demonstrating that the species exists on a time scale longer than 10 microseconds. The appearance potential for HS(2+) from H,S is 42.3 + or - 1.0eV. Evidence is also presented for the electron impact production of S(2+), H2S(2+) and H3S(2+).

100 296 PB91-148940 Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Fire Measurement and Research Div.

Applicability of Smoluchowski's Equation with a Constant Kernel to Coalescence.

G. W. Mulholland, and R. D. Mountain. 1986, 2p Pub. in Jnl. of Chemical Physics 84, n7 p4109-4110, 1 Apr 86.

Keywords: \*Coalescence, Computerized simulation, Reprints, \*Smoluchowski equation.

A computer simulation of particle size independent coagulation is carried out to test the applicability of Smoluchowski's coagulation theory for coalescence. A small time enhancement in the coagulation rate is observed for the simulation. A straightforward generalization of the coagulation theory to include a transient term does not yield results in quantitative agreement with the simulation.

100.297 PB91-148973 Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Quantum Physics Div. H + O3 Fourier-Transform Infrared Emission and

Laser Absorption Studies of OH (X(2) Pi) Radical: An Experimental Dipole Moment Function and State-to-State Einstein A Coefficients.

D. D. Nelson, A. Schiffman, D. J. Nesbitt, J. J. Orlando, and J. B. Burkholder. 1990, 17p Contract AFOSR-F49620-86-C-0056

Sponsored by Air Force Office of Scientific Research,

Bolling AFB, DC.
Pub. in Jnl. of Chemical Physics **9**3, n10 p7003-7019, 15 Nov 90.

Keywords: \*Hydroxyl radicals, Vibrational spectra, Dipole moments, Einstein coefficients, Atmospheric radiation, Reprints, Fourier transform infrared spec-

The relative intensities of 88 pairs of rovibrational transitions of OH (X (Sup 2) Pi) distributed over 16 vibrational bands (nu prime < 9, delta nu = -1, -2) have been measured using Fourier transform infrared (FTIR) emission/absorption spectroscopy. Each pair of transitions originates from a common vibrational, rotations. tational, and spin-orbit state, so that the measured relative intensities are independent of the OH number density and guantum state distribution. These data are combined with previous nu = 1 < 0 relative intestig absorption measurements and nu = 0, 1, and 2 permanent dipole moments to determine the OH dipole moment function as a cubic polynomial expanded about the equilibrium bond length. The relative intensities provide detailed information about the shape of the OH dipole moment function mu(r) and hence the absolute Einstein A coefficients. Absolute Einstein A coefficients from the present mu(r) are therefore presented in order to provide the most reliable experimental numbers for modeling of near IR atmosphere OH emission phenomena.

100,298

PB91-149005 Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Quantum Physics Div.

Laser-Induced Fluorescence Measurements of Drift-Velocity Distributions for Ba(+) in Ar:

Moment Analysis and a Direct Measure of Skewness.

Final rept.

S. M. Penn, J. P. M. Beijers, R. A. Dressler, V. M. Bierbaum, and S. R. Leone. 1990, 10p Contract AFOSR84-02

Sponsored by Air Force Office of Scientific Research,

Bolling AFB, DC Pub. in Jnl. of Chemical Physics 93, n7 p5118-5127, 1 Oct 90.

Keywords: \*Barium ions, Laser induced fluorescence, lon mobility, Ion temperature, Velocity distribution, Doppler effect, Skewness, Argon, Drift, Reprints.

Velocity distributions for Ba(1+) ions drifting in argon under the influence of an electric field are measured using single-frequency, laser-induced fluorescence techniques. A moment analysis of these data yields values for the ion mobilities, temperatures, and, for the first time, skewness parameters of the ion velocity distributions. Doppler profiles of the drifting ions are obtained with the laser beam propagating both parallel and perpendicular to the electric field direction as a function of E/N up to 148 Td.

100,299

PB91-149161 Not available NTIS ing.

Final rept. S. R. Rudge, and P. Todd. 1990, 27p

Pub. in Protein Purification from Molecular Mechanisms to Large-Scale Processes, ACS Symposium Series 427, Chapter 16, p244-270 1990.

Keywords: \*Ions, \*Interfaces, \*Electric fields, Thermodynamics, Electrolytes, Electrophonesis, Reviews, Proteins, Reprints, \*lonic partitioning.

Electric potentials at interfaces are governed by the distribution of ions between the phases. The fundamental thermodynamics of ionic partitioning are reviewed, and the implications of the resulting double layer for transport processes in electric fields are discussed. The special considerations of electric field applications, concerning heat and mass transport, are presented. Electric fields have been applied to aqueous biphasic demixing and to cell separations by density gradient electrophoresis and free flow electrophoresis, for the purpose of producing gram quantities of protein. Analytical applications of electric fields, for the purpose of monitoring downstream processes, have also been successful. These applications include capillary electrophoresis, electrospray mass spectrometry, and pulsed field electrophoresis.

100,300

Not available NTIS PB91-149369 National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.

Influence of Sulfur on Methanation over Tungsten(110). Final rept

P. D. Szuromi, R. D. Kelley, and T. E. Madey. 1986,

Pub. in Jnl. of Physical Chemistry 90, n24 p6499-6507 1986

Keywords: \*Sulfur, \*Tungsten, \*Reaction kinetics, \*Surface chemistry, \*Catalysts, Carbon monoxide, Hydrogen, Oxygen, Auger electron spectroscopy, Clumps, Activation energy, Methane, Reprints, \*Methane, Rep

The effect of adsorbed sulfur on the rate of methanation over W(110) is reported for a range of sulfur coverages (0.03-0.55 mL) and temperatures (600-750K) for Torr CO and 100 Torr hydrogen. The rate drops sharply for low sulfur coverages (by 40% at 0.05 mL) but decreases less dramatically for higher coverages. Postreaction Auger spectra reveal that the sulfur-free surface for the sample is covered with both carbidic carbon and oxygen, and is oxygen rich. Increasing

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sulfur coverages leads to little change in the postreaction carbon level but does cause the oxygen coverage to fall substantially, to zero by 0.40 ml S. The activation energy for methanation is unaffected by the presence of sulfur, suggesting that the decrease in rate is caused by sulfur limiting the saturation coverages that can be attained by the reactants. This possibility motivated a thermal desorption study of CO and hydrogen adsorption on sulfur precovered surfaces. Good agreement is obtained between the changes in these saturation coverages and the decrease in methanation rate due to the presence of sulfur when small coverages of coadsorbed oxygen are present. These results taken as a whole suggest that sulfur adatoms inhibit methanation through long-range effects, which appear to be moderated by the formation of clusters. Such cluster formation is itself inhibited at low sulfur coverages by the presence of oxygen, which causes sulfur to poison the reaction more effectively at such low coverages.

100,301 PB91-149377 PB91-149377 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.
Summary Abstract: The Influence of Sulfur on Methanation over W(110).

Final rept. P. D. Szuromi, R. D. Kelley, and T. E. Madey. 1987,

2p Pub. in Jnl. of Vacuum Science and Technology A 5,

Keywords: \*Sulfur, \*Tungsten, \*Reaction kinetics, \*Surface chemistry, \*Catalysts, Carbon monoxide, Hydrogen, Oxygen, Auger electron spectroscopy, Clumps, Activation energy, Methane, Reprints, \*Methanation.

The effect of adsorbed sulfur on the rate of methanation over W(110) is reported for a range of sulfur cover-ages (0.03-0.55 mL) and temperatures (600-750K) for 1 Torr CO and 100 Torr hydrogen. The rate drops sharply for low sulfur coverages (by 40% at 0.05 mL) but decreases less dramatically for higher coverages. Postreaction Auger spectra reveal that the sulfur-free surface for the sample is covered with both carbidic carbon and oxygen, and is oxygen rich. Increasing sulfur coverages leads to little change in the postreaction carbon level but does cause the oxygen coverage. to fall substantially, to zero by 0.40 mL of S. The activation energy for methanation is unaffected by the presence of sulfur, suggesting that the decrease in rate is caused by sulfur limiting the saturation coverages that can be attained by the reactants. This possibility motivated a thermal desorption study of CO and hydrogen adsorption on sulfur precovered surfaces. Good agreement is obtained between the changes in these saturation coverages and the decrease in meth-anation rate due to the presence of sulfur when small coverages of coadsorbed oxygen are present. These results taken as a whole suggest that sulfur adatoms inhibit methanation through long-range effects, which appear to be moderated by the formation of clusters. Such cluster formation is itself inhibited at low sulfur coverages by the presence of oxygen, which causes sulfur to poison the reaction more effectively at such low coverages.

100,302 PB91-149385 Not available NTIS

Not available NTI National Inst. of Standards and Technology (NML), Boulder, CO. Quantum Physics Div.

General Method for Doppler Determination of Cylindrically Symmetric Velocity Distributions: An Application of Fourier Transform Doppler Spectroscopy. Final rept.

C. A. Taatjes, J. I. Cline, and S. R. Leone. 1990, 6p Grant NSF-PHY86-04504

Sponsored by National Science Foundation, Washington, DC., and Air Force Weapons Lab., Kirtland AFB, NM.

Pub. in Jnl. of Chemical Physics 93, n9 p6554-6559, 1 Nov 90.

Keywords: Velocity distribution, Doppler effect, Hermite polynomials, Anisotropy, Reprints, \*lodine atoms, Fourier transform Doppler spectroscopy

A general method is developed for determination of cylindrically symmetric velocity distributions from Doppler profile measurements. The method applies Kinsey's Fourier transform Doppler spectroscopy Kinsey, J. Chem. Phys. 66,2560 (1977)) to distributions arising from photodissociation and uses an orthogonal polynomial expansion to perform the integral transforms analytically. The method is shown to offer an improvement in stability over direct numerical solution of the integral equation and to have applicability to distri-butions which are not 'separable,' that is, which cannot be separated into a product of speed- and angle-dependent factors. The method is applied to experimental measurements of the collisional relaxation of a fast anisotropic distribution of I(doublet P(1/2)) atoms in a thermal bath. It is shown that the nascent distribution is separable, but the distribution does not remain separable throughout the relaxation process.

PB91-149393

Not available NTIS National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Ceramics Div.

Relation between the Surface Energy and the Debye Temperature for Cubic Solids.

V. K. Tewary, and E. R. Fuller. 1990, 5p Pub. in Jnl. of Materials Research 5, n5 p1118-1122

Keywords: \*Specific heat, \*Surface energy, \*Simple cubic lattices, \*Solids, Atomic mass, Reprints.

It is shown that a phenomenological relation exists between the Debye temperature theta (in degree Kelvin) and the surface energy Gamma (in ergs/sq cm) of cubic solids: theta = (71.9)(Gamma/M)(sup 1/2), where M is the atomic weight. This relation is derived theoretically in the Debye isotropic approximation by assuming that the interatomic potential is central. No restrictions are imposed on the range of the potential. The relation is obeyed very well by the observed values of theta and gamma in the case of many solids.

PB91-149831 Not available NTIS National Bureau of Standards (NEL), Boulder, CO. Chemical Engineering Science Div.
Thermodynamics of Ammonium Indates. 2. The

Molar Heat Capacity of the Ammonium Pentabro-moindate Monohydrate Salt (NH4)2 InBr5.H2O from 7.8 to 348 K. Final rept.

S. M. Acosta, E. F. Westrum, R. J. C. Brown, J. E. Callanan, and R. D. Weir. 1988, 6p See also PB89-123905.

Pub. in Jnl. of Chemical Thermodynamics 20, p1321-1326 1988

Keywords: \*Indium inorganic compounds, \*Specific heat, Calorimetry, Adiabatic conditions, Reprints, \*Ammonium pentabromoindate monohydrate.

The molar heat capacity of ammonium pentabromoindate monohydrate (NH4)2InBr5 - H2O was measured from 7.8 to 348 K using adiabatic calorimetry. The curve of heat capacity as a function of temperature is continuous. There is no sign of the phase transition predicted by Yamada and Weiss (Ber. Bunsenges. Phys Chem. 1983, 87, 932). Values of the standard molar thermodynamic quantities for (NH4)2InBr5 H2O are presented to 345 K.

100 305

Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Chemical Engineering Science Div. Thermodynamics of the Divalent Metal Fluorides.

3. Heat Capacity of the Fast Ion Conductor Sr SnF4 from 6 to 344 K. Not available NTIS PB91-149864

Final rept. J. E. Callanan, R. Shaviv, E. F. Westrum, and R. D. Weir. 1989, 7p See also PB91-133850.

Pub. in Jnl. of Solid State Chemistry 81, p51-57 1989.

Keywords: \*Specific heat, Ionic conductivity, Temperature dependence, Reprints, \*Strontium tin fluorides, \*Strontium tetrafluorostannates.

The heat capacity of the fast ion conductor SrSnF4 was measured by adiabatic calorimetry from 6 < T/K < 344. A phase transition was not detected, but an anomalous rise in the molar heat capacity was found above 280 K that showed no sign of lessening at 344 K. The rise is coincident with the temperature range where a rapid drop in the (19)F spin-lattice relaxation time T(1) occurs. Standard molar thermodynamic func-tions are given at selected temperatures from 5 to 345 100,306

PB91-149906 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Molecular Physics Div. Vibrational Spectra of Molecular Ions Isolated in Solid Neon. 5. N2O(1+) and NNO2(1-).

Final rept.

M. E. Jacox. 1990, 10p See also PB91-149914 and PB91-112714. Sponsored by Army Research Office, Research Triangle Park, NC. Pub. in Jnl. of Chemical Physics 93, n11 p7622-7631, 1

Keywords: \*Molecular ions, \*Nitrous oxide, \*Vibrational spectra, Matrix isolation, Infrared spectra, Solidified gases, Penning effect, Absorption spectra, Photoionistics, Pho zation, Photolysis, Cryogenics, Reprints, Solid neon.

When a Ne:N2O = 200 or 800 sample is codeposited at approximately 5 K with a beam of neon atoms that has been excited in a microwave discharge, the infrared spectrum of the products includes absorptions contributed by the two stretching fundamentals of ground-state N2O(H). An abosrption near 1200/cm also results from the stabilization of NNO2(1-) on reaction of O(1-) with N2O. The two other stretching fundamentals of NNO2 have also been identified. Detailed isotopic substitution studies support these identificaisotopic substitution studies support these internitica-tions and permit a normal coordinate analysis for both N2O(1+) and NNO2. The nitrogen-nitrogen bond of NNO2(1-) has approximately single bond character, and the nitrogen-oxygen bonds are relatively weak. The photodestruction threshold for NNO2 in this ex-perimental system is near 420 nm. Photolysis of NNO2(1-) is accompanied by growth in the absence NNO2(1-) is accompanied by growth in the absorptions of cis ONNO. Several other infrared absorptions in the initial sample are tentatively assigned to vibrations of N2O complexed to various ions.

100,307

PB91-149914 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Molecular Physics Div.

Vibrational Spectra of Molecular Ions Isolated in Solid Neon. 4. NO(1+), NO(1-), ONNO(1+), and ONNO(1-).

Final rept.

M. E. Jacox, and W. E. Thompson. 1990, 13p See also PB91-149906 and PB91-112714. Sponsored by Army Research Office, Research Triangle Park, NC. Pub. in Jnl. of Chemical Physics 93, n11 p7609-7621, 1 Dec 90.

Keywords: \*Molecular ions, \*Nitric oxide, \*Vibrational spectra, Matrix isolation, Solidified gases, Photoionization, Photolysis, Infrared spectra, Penning effect, Cryogenics, Reprints, Solid neon.

When a Ne:NO sample is codeposited at approximately 5 K with a beam of neon atoms that has been excited in a microwave discharge, photoionization and Penning ionization of the NO lead to the stabilization of both monomer and dimer ions. The most prominent infrared absorption, at 1619.2/cm, results from the reacfrared absorption, at 1619.2/cm, results from the reaction of NO with NO or of an electron with (NO)2 to form the charge-delocalized trans-ONNO(1-) species. The position of the totally symmetric NO-stretching absorption of trans ONNO(1-) can be inferred from observation of a combination band. The infrared absorption of NO(1+) has been detected very close to the gasphase band center. Other infrared absorptions have been tentatively assigned to NO, cis ONNO(1+), trans ONNO, and the lowest energy isomer of ONNO(1+). Comparison of the gas-phase vibrational frequencies observed for the weakly bound species cis ONNO and observed for the weakly bound species cis ONNO and N2O3 with the corresponding frequencies observed in this neon-matrix study suggests that the matrix shifts for the dimer ion absorptions in the mid-infrared probably amount to less than 1%.

100.308

PB91-149955 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Molecular Physics Div.

Application of Ultrafast Broadband Infrared Spectroscopy to Measurement of Metal-Carbonyl Dynamics.

S. A. Angel, P. A. Hansen, E. J. Heilweil, and J. C. Stephenson. 1990, 3p Pub. in Springer Series in Chemical Physics, v53 p480-

Keywords: \*Metal carbonyls, Carbon monoxide, Nitric oxide, Infrared spectra, Picosecond pulses, Liquid phases, Vapor phases, Vibrational spectra, Reprints.

Population lifetimes and energy transfer dynamics obtained from transient multichannel infrared spectra of CO and NO (v=1) vibrations for gas and liquid phase metal-carbonyl systems are presented.

100,309

PB91-150003 Not available NTIS National Inst. of Standards and Technology (NEL), Boulder, CO. Chemical Engineering Science Div.

Fusion of Mercury. A New Certified Standard for Differential Scanning Calorimetry

Final rept. J. E. Callanan, K. M. McDermott, and E. F. Westrum.

1990, 6p Pub. in Jnl. of Chemical Thermodynamics 22, p225-

Keywords: \*Mercury, \*Heat of fusion, \*Melting points, \*Standards, \*Differential thermal analysis, Calorimetry, Adiabatic conditions, Reprints.

From the results of adiabatic-calorimetric measurements, mercury has been certified as a standard reference material for temperature and enthalpy of fusion for differential scanning calorimetry. The fusion temperature is (234.30 + or - 0.03) K and the molar enthalpy of fusion is (2.301 + or - 0.001) kJ per mole. Adiabatic-calorimetric measurements made by heating continuously at 0.00017 K per second through the transition showed a fusion temperature of (234.32 + or - 0.03)K. Differential-scanning-calorimetric measurements gave a fusion temperature of (234.34 + or -0.48)K.

100,310 PB91-150052 Not available NTIS National Inst. of Standards and Technology (NML),

Boulder, CO. Quantum Physics Div.

Diode Laser Probing of I\*((2)P1/2) Doppler Profiles: Time Evolution of a Fast, Anisotropic Velocity Distribution in a Thermal Bath.

J. I. Cline, C. A. Taatjes, and S. R. Leone. 1990, 11p Sponsored by Weapons Lab., Kirtland AFB, NM. ub. in Jnl. of Chemical Physics 93, n9 p6543-6553, 1

Keywords: Velocity distribution, Doppler effect, Infra-red spectra, Anisotropy, Reprints, \*Iodine atoms.

The relaxation of a nonthermal translational population distribution of fast I\* (doublet P(1/2)) atoms dilutely dispersed in a gaseous bath at thermal equilibrium is studied by time-resolved Doppler spectroscopy. The fast, anisotropic velocity distribution of 1\* atoms is produced by pulsed laser photolysis of n-perfluoropropyl iodide (n-C3F7I) at 266 nm. A frequency-narrowed, GaAsInP diod e laser is tuned across the iodine transition at 1315 nm to measure the Doppler gain profile of the I\* photofragments. The velocity distribution is expressed as a separable product of a radial speed function and an angular function describing the anisotropy. The collision-induced time evolution of both the speed and anisotropy components of the nascent velocity population distribution relaxing to form a 300 K Maxwellian equilibrium distribution is determined.

PB91-158717 Not available NTIS National Inst. of Standards and Technology (IMSE), Gaithersburg, MD. Reactor Radiation Div.

New Different Forms of Ammonium Loaded and

Partly Deammoniated Zeolite Rho Studied by Neutron Powder.

Final rept. R. Fischer, W. Baur, R. Shannon, J. Parise, and J. Faber, 1989, 7p

Pub. in Acta Cryst. C45, p983-989 1989.

Keywords: \*Zeolites, \*Ion exchange resins, Crystal Neutron diffraction, Powder(Particles), Simple cubic latties, Deuteration, Calcines, Roasting, Cesium compounds, Aluminum compounds, Inorganic silicates, Ions, Reprints, Zeolite RHO, Rietveld method.

Zeolite ND4-Rho, prepared by shallow-bed calcination of ammonium-exchanged Rho under flowing dry nitrogen at 873 K, subsequently reloaded with ammonium, deuterium exchanged and D2.5(ND4)7.4Cs0.7Al10.9Si37.1O96, dehydrated: M(sub D2.5(ND4)7.4Cs0.7Al10.9Si37.1O96, M(sub r) = 3073.45, cubic, I43m, a = 14.5265(7)A, V = 3065.37 cu

A, Z=1, Dx=1.685 g/cc, Reitveld refined refinement based on time-of-flight neutron powder diffraction data collected at room temperature. Zeolite ND4-Rho, prepared by deep-bed calcination of ammonium-exchanged Rho in air at 633 K, yielding a partly deammoniated sample, subsequently deuterium exchanged and dehydrated: Dx(ND4)4.6Cs0.55Al10.1Si37.9-O96, M(sub r) = 3047.28, cubic, 143m, a = 14.4247(5)A, V = 3001.38 cuA, Z = 1, Dx = 1.685 g/cc, Rietveld refinement based on fixed-wavelength neutron powder diffraction data collected at room temperature, lambda = 1.5423(6)A.

PB91-158790 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Chemical Kinetics Div.

Zonal Model for Corona Discharge-Induced Oxidation of SF6 in SF6/O2/H2O Gas Mixtures. Final rept.

J. T. Herron, and R. J. Van Brunt. 1989, 6p Sponsored by Department of Energy, Washington, DC. Pub. in Proceedings of International Symposium on Plasma Chemistry (9th), Pugnochiuso, Italy, September 4-8, 1989, v1 p257-262.

Keywords: \*Sulfur hexafluoride, \*Reaction kinetics, \*Oxidation, \*Corona discharges, \*Mathematical models, Oxygen, Oxygen fluorides, Mixtures, Water vapor, Reprints.

A chemical kinetics model for oxidation of SF6 in negative glow-type corona discharges is proposed. The model is applied to highly localized dc, point-plane negative corona discharges in SF6/O2 mixtures containing water vapor, and resulting predictions for oxidation by-product yields are compared with recent data on rates for SOF2, SOF4, SO2F2, SO2, and S2F10 formation from corona discharges in SF6 and SF6/O2 mixtures.

PB91-158857 Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Thermophysics Div. Wetting Layers on Solid Substrates. Final rept.

R. F. Kayser. 1987, 19p Pub. in KINAM, v8 ptA p87-105 1987.

Keywords: \*Wetting, Wettability, Substrates, Glass, Dispersion, Reprints, Ionic forces.

When two fluids coexist near a substrate, a thin layer of one fluid often intrudes between the other fluid and the substrate. The thickness of such an intruding layer is often determined by a competition between gravitational forces, which tend to thin the layer, and longrange dispersion forces, which tend to thicken the layer. The paper reviews the theory of wetting layers stabilized by dispersion forces and delimits the applicability of the theory. It also presents a new derivation of the wetting layer thickness for wetting layers stabilized by ionic forces. The mechanism differs from that of dispersion forces and arises when a solid surface can become electrically charged. Elements of both theories are needed to explain recent measurements of wetting layers on glass.

PB91-161927 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Surface Science Div. Picosecond IR Studies of the Vibrational Dynamics of CO/Pt(111).

Final rept.
J. D. Beckerle, M. P. Casassa, E. J. Heilweil, R. R. Cavanagh, and J. C. Stephenson. 1990, 10p Sponsored by Air Force Office of Scientific Research, Bolling AFB, DC.

Pub. in Jnl. of Electron Spectroscopy and Related Phenomena 54/55, p17-26 1990.

Keywords: \*Carbon monoxide, \*Vibrational states, Vibrational spectra, Infrared spectroscopy, Picosecond pulses, Chemisorption, Platinum, Surfaces, Reprints.

vibrational dynamics of chemisorbed CO on Pt(111) are investigated by picosecond IR transient saturation spectroscopy. An intense ps pump pulse excites the CO stretch vibration for CO/Pt(111) and the transient differential IR spectrum of the vibrationally excited adlayer is monitored with a second IR probe pulse. The transient spectrum exhibits a dispersive bandshape, with both bleach and absorption features. The transient spectrum appears prior to the pump pulse and decays within a few ps following the pump pulse. The results are interpreted by comparison with analogous measurements on metal carbonyl molecules, and model calculations including the effects of optical coherence.

100.315

PB91-161968 Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Thermodynamics Div.

Research at NBS on Dynamic Measurements of Thermophysical Properties at High Temperature (Abstract).

Final rept.

A. Cezairliyan, 1988, 1p

Pub. in Thermal Conductivity, p3 1988.

Keywords: \*Thermophysical properties, Electric conductors, High temperature, Reduced gravity, Measurement, US NBS, Reprints.

Techniques will be described for the dynamic measurements of selected thermophysical properties of electrically conducting substances at temperatures above 1500 K and up to about 10,000 K. The techniques are based on rapid resistive self-heating of the specimen from room temperature to any desired high temperature in less than one second by the passage of an electrical current pulse through it and on measuring the pertinent quantities with appropriate time resolu-tion. Both millisecond and microsecond resolution techniques developed at NBS will be described, and examples of measured properties will be given. The potential applications of the technique, including property measurements in a microgravity environment, will be discussed.

100,316

PB91-162057 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Molecular Physics Div. H2O2: Spectroscopy, Structure and Dynamics. Final rept.

G. T. Fraser. 1991, 18p Pub. in International Review in Physical Chemistry 10, n2 p189-206 1991.

Keywords: \*Water, \*Dimerization, \*Hydrogen bonds, Electron tunneling, Molecular structure, Molecular spectroscopy, Reprints.

Tunnelling in water dimer allows each of the hydrogen atoms to participate in the hydrogen bonding, giving rise to a complicated energy-level scheme and rotational spectrum. As a result of new theoretical and experimental developments, great progress has been made in the analysis and interpretation of the spectrum, yielding detailed information about this hydrogen-bonded interaction. The paper reviews the spectroscopy of the highly non-rigid dimer, which is becoming a prototype system for the study of multidimensional tunnelling problems in weakly bound complex-

100,317

PB91-162065 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Surface Science Div.
Resonant Tunneling with Electron-Phonon Interactions: An Exactly Solvable Model Applied to De-

sorption. Final rept.

J. W. Gadzuk. 1990, 10p

Pub. in Jnl. of Electron Spectroscopy and Related Phenomena 54/55, p201-210 1990.

Keywords: \*Resonant tunneling, \*Desorption, Electron phonon interactions, Electron tunneling, Hot electrons, Surface reactions, Molecules, Atoms, Reprints, Laser induced desorption, Quantum wells.

The problem of hot electron and/or laser induced desorption of atoms or molecules on surfaces is considered. The equivalence between a previous wavepacket model for this process and the problem of inelastic resonant electron tunneling through a quantum well with electron-phonon coupling is established. Numerical consequences of some exactly solved quantum well models are explored as they relate to desorption.

100,318

PB91-162073

Not available NTIS

# **Physical & Theoretical Chemistry**

National Inst. of Standards and Technology (NML), Boulder, CO. Thermophysics Div.

Phase Transitions.

Final rept. M. S. Green, and J. M. H. Levelt Sengers. 1990, 5p Pub. in Encyclopedia of Physics, p897-901 1990.

Keywords: \*Phase transformations, Order disorder transformations, Phase diagrams, Phase rule, Liquid crystals, Ising model, Order parameters, Reprints, Lat-

The report is an update of the original Article on Phase Transitions written by M. S. Green. Several phase trans sitions have been added to the ones covered by M. S. Green. The presentations of the concepts of order-dis-order phenomena, order parameter and critical-point universality have been expanded and updated. Illustrations have been improved and new ones added.

100.319 PB91-162081 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Thermophysics Div. Unified Description of Infinite-Dilution Thermody-

namic Properties for Aqueous Solutes. Final rept.

A. H. Harvey, J. M. H. Levelt Sengers, and J. C. Tanger. 1991, 6p Pub. in Jnl. of Physical Chemistry 95, n2 p932-937

Keywords: \*Solubility, \*Henrys law, \*Argon, \*Xenon, \*Ethylene, \*Specific heat, \*Aqueous solutions, Critical point, Density(Mass/volume), Thermodynamics, Analysis(Mathematics), Reprints, \*Infinite dilution, \*Infinite dilution,

A linear expression, asymptotically correct near a solvent's critical point, is derived relating Henry's constant of a solute to the density of the pure solvent. Since the expression is general (i.e. not restricted to the solvent's saturation curve), it may be differentiated to yield other infinite-dilution thermodynamic properties such as partial molar volumes. This enables these properties for a solute to be predicted from a single fit of the Henry's constant expression to solubility data. Such predictions are compared with published measurements of apparent molar volumes and a apparent molar heat capacities for aqueous argon, xenon, and ethylene. The volumes are predicted well over a wide range of conditions including the region near water's critical point, where large effects are observed. Agreement with heat capacity data is only qualitative, the authors show that this may be in part a consequence of a higher order term in the asymptotic expression that be-comes important after two differentiations. The divergent behavior of the infinite-dilution properties near the critical point is determined by divergences in pure-solvent properties; the only solute dependence is in the amplitude of the divergence, which is proportional to the slope of the Henry's constant expression. While the experimental Henry's constant data yield a very large linear region, it now appears that the slope in the region is not the true asymptotic slope. Nevertheless, it appears that predictions of infinite-dilution thermodynamic properties based on Henry's constants are adequate over a wide range of conditions.

100,320 PB91-162289 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Surface Science Div. Surface-State-Mediated Photochemistry: Laser-Induced Desorption of NO from Si (111).

L. J. Richter, S. A. Buntin, D. S. King, and R. R. Cavanagh. 1990, 4p Contract DE-AI05-84ER13150

Sponsored by Department of Energy, Washington, DC. Pub. in Physical Review Letters 65, n15 p1957-1960, 8

Keywords: \*Nitric oxide, \*Desorption, Chemisorption, Surface chemistry, Silicon, Lasers, Reprints.

Laser-induced desorption of NO from Si(111) has been investigated using state-specific detection techniques. Characterization of the internal-state population distributions with desorption-laser wavelengths in the range 1907-355 nm indicate that, at low initial NO coverages, desorption is driven by a common, nonthermal mechanism. The wavelength dependence of the yield and the effects of coadsorbates on the yield es-tablish that photogenerated holes in a Si intrinsic sur-face state mediate the laser-adsorbate interaction.

100,321 PB91-167213 PC A05/MF A01 National Inst. of Standards and Technology, Gaithersburg, MD. Technical Activities 1990, Standard Reference

Data Program. M. W. Chase. Jan 91, 83p NISTIR-4505 See also PB90-185109.

Keywords: Physical properties, Chemical properties, Thermodynamics, Materials, Data bases, \*Chemical information systems, \*Standard reference data, US NIST, NSRDS system.

Standard Reference Data is a program office within the Office of Measurement Services in Technology Services, National Institute of Standards and Technology. Standard Reference Data develops and dissemi-nates publications and databases of critically evaluated physical, chemical, and materials properties of substances. These publications and databases are available through NIST and private publishers, on magnetic tape and PC diskettes, and from online retrieval systems. Standard Reference Data is responsible for management and coordination of the program. Work is carried out through a decentralized network of data centers and projects referred to as the National Standard Reference Data System (NSRDS). The volume summarizes the activities of the program for the fiscal

100,322 PB91-174763 Not available NTIS National Inst. of Standards and Technology (NEL), Boulder, CO. Thermophysics Div. Viscosity Surface for Mixtures of Methane and Ethane. Final rept.

D. G. Friend. 1990, 8p Pub. in Cryogenics 30, p105-112 Feb 90.

Keywords: \*Ethane, \*Methane, \*Viscosity, \*Binary mixtures, Fluids, Physical properties, Experimental data, Statistical analysis, Reprints.

The viscosity surface for methane-ethane mixtures has been correlated as a function of composition, density and temperature. The correlation is based on measurements, made at the National Institute of Standards and Technology, using a torsionally oscillating quartz crystal viscometer, which have been reported previously. The viscosity data cover the composition range including both pure fluids and three of their binary mixtures and include temperatures from 100 to 320 K with pressures to 30 MPa. The correlation com-prises contributions from the dilute gas state, based entirely on Chapman-Enskog mixture theory and an empirical excess function. The excess function exploits corresponding states arguments and, with suitable reductions of the viscosity, density and temperature, the data are seen to conform closely to a single function of the reduced quantities. The very steep rise of viscosity at high densities is described by a simple rational polynomial and this is added to another polynomial in reduced density and temperature to completely represent the reduced excess viscosity. For the 624 experimental points which were considered, the average absolute deviation from the correlation is less than 1.5%.

PB91-174805 Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Chemical Engineering Science Div. Increased Facilitated Transport Related to Microstructural Changes in Heat-Treated Ion-Exchange Membranes.

M. D. Heaney, and J. J. Pellegrino. 1989, 19p Sponsored by Department of Energy, Morgantown, WV. Morgantown Energy Technology Center. Pub. in Jnl. of Membrane Science 47, p143-161 1989.

Keywords: \*lon exchange materials, \*Membrane transport, \*Membranes, Microstructure, Heating, Temperature dependence, Hydrophylic polymers, Perfluoro compounds, Polymeric films, Swelling, Corrosive gases, Permeability, Small angle scattering, Carbon dioxide, Separation processes, Reprints, Ionomers.

Poly(perfluorosulfonic acid) ionomer films were subjected to a heat treatment, with a low volatility polar solvent, which swells the film. These swollen films were used as supports for liquid membranes using

water as a solvent. The diffusive and facilitated transport of acid gases was measured and found to be greatly increased in these membranes versus untreated ones. Microstructural analysis of the films, using small angle X-ray scattering, indicates that there is an increase in the size of the ionic (hydrophilic) clusters. The increase in ionic cluster size correlates with the observed increase in permeability of the acid gases. The effective diffusion coefficient of the carbon dioxide carrier complex (determined from a model for facilitated transport) has increased by 1-2 orders of magnitude, while that of the carbon dioxide alone has increased only 4-fold over the same range of heat treat-ment conditions. The microstructural changes persist over extended periods of time, and therefore the heat treatment is possibly a practical means of increasing permeability for this polymer in commercial applica-tions. In limited tests it has been previously confirmed that the selectivity of the treated membranes for carbon dioxide versus carbon monoxide remains high, with separation factors of 126 to 70.

100,324 PB91-174813 Not available NTIS Not available NTS National Bureau of Standards (NML), Gaithersburg, MD. Molecular Spectroscopy Div.

Population Lifetimes of OH (v=1) and OD (v=1) Vibrations in Alcohols, Silanols and Crystalline

Micas.

Final rept.

E. J. Heilweil, M. P. Cassassa, R. R. Cavanagh, and J. C. Stephenson. 1986, 4p Sponsored by Air Force Office of Scientific Research,

Bolling AFB, DC.
Pub. in Springer Series in Chemical Physics 'Ultrafast Phenomena V', v46 p465-468 1986.

Keywords: \*Vibrational states, \*Alcohols, \*Mica, Silanes, Deuterium compounds, Chemical bonds, Electronic states, Lifetime, Reprints, Hydroxy group, Silan-

Vibrational energy dynamics of excited fundamental modes of ground electronic state condensed-phase molecules is suspected of playing a role in many bondbreaking physical and chemical processes. As a first step in elucidating this role, it is necessary to compare the vibrational v=1 lifetimes (T sub 1) of a specific functional group in a variety of molecules and chemical environments. It should then be possible to determine whether structural or other vibrational properties of a molecular family influence that particular group's chemical reactivity.

100 325 PB91-174821 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Chemical Kinetics Div.

Thermochemistry of Sulfoxides and Sulfones. Final rept. T. Herron. 1988, 12p

Pub. in Chem. Sulphones Sulphoxides, p95-106 1988. Keywords: \*Sulfoxides, \*Sulfones, \*Sulfates, \*Sulfites, \*Thermochemical properties, Experimental data, Reviews, Reprints, Chemical structure.

The report is a review of the experimental data on the thermochemistry of sulfoxides, sulfones, sulfites, and sulfates, and the use of such data in developing esti-mation methods, deriving bond strengths, and inter-preting data on the thermal stability and chemical kinetics of these species. Group values are presented for the estimation of thermochemical properties using the method of group additivity.

PB91-174839 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Chemical Kinetics Div. Formation and Stability of SF5 and S2F10. Final rept.

J. T. Herron, and W. Tsang. 1987, 6p Pub. in Proceedings of International Symposium on Gaseous Dielectrics (5th), p199-204 1987.

Keywords: \*Sulfur fluorides, \*Sulfur hexafluoride, \*Di-electric properties, \*Thermal stability, Thermodynamic properties, Reaction kinetics, Water vapor, Computerized simulation, Reprints.

The simulation of the dielectric breakdown of SF6 through the use of computer modeling offers many advantages over more costly direct testing methods for determining the conditions under which potentially

toxic by-products may be generated. A complete model calculation requires a knowledge of the rate constants or cross sections for all relevant processes. A complete data base of that nature has not yet been assembled. However enough data exist to begin to answer some of the pressing questions regarding the formation and stability of various proposed reaction in-termediates. Computer modeling studies have been carried out for very simple systems in order to determine the conditions under which S2F10 is formed and the role of water vapor in that process. Many other recombination products of undetermined toxicity such as S2F4, S2F6, and S2F8 can be formed following the breakdown of SF6. The thermal stability of SF5 and S2F10 is discussed and the lifetimes of these species given as a function of temperature.

100,327 PB91-174847 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Chemical Kinetics Div. Letter to Editor of Chemical and Engineering

News. Final rept.

J. T. Herron, and W. Tsang. 1987, 1p

Pub. in Chemical and Engineering News 65, n44 p3

Keywords: \*Combustion, Chemical reactions, Reaction kinetics, Reprints.

This is a one-page letter to the editor of Chemical and Engineering News, on the subject of combustion chemistry.

100,328 PB91-174870 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Chemical Kinetics Div.

Resonance Enhanced Multiphoton Ionization Spectroscopy of CHCI2 and CDCI2.

J. W. Hudgens, and G. R. Long. 1988, 3p Pub. in AIP Conference Proceedings, n172 p337-339

Keywords: \*Electronic spectra, \*Ionization, Spectrum analysis, Spectral lines, Free radicals, Isotope effect, Molecular vibration, Reprints, \*Chloromethyl radicals, Purbless et test Rydberg states.

Resonance enhanced multiphoton ionization spectra of CHCl2 and CDCl2 were observed between 355-375 nanometers (nm) via a 2 + 1 excitation process. Electronic origins tentatively assigned to 3d Rydberg states were observed at 370.1 nm (frequency = 54,024 per cm) for CHCl2 and at 370.4 nm (frequency = 53,980 per cm) for CDCl2. The C-Cl symmetric stretch frequencies are 845 per cm in CHCl2 and 814 per cm in

100,329 PB91-174995 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Quantum Metrology Div.

Polarized X-ray Emission Studies of Methyl Chloride and the Chlorofluoromethanes.

D. W. Lindle, P. L. Cowan, T. Jach, R. E. LaVilla, R. D. Deslattes, and R. C. C. Perera. 1991, 14p Sponsored by Department of Energy, Washington, DC. Pub. in Physical Review A 43, n5 p2353-2366, 1 Mar

Keywords: \*Chloromethanes, \*Methyl chloride, \*Di-chlorodifluoromethane, Polarization(Waves), Synchrotron radiation, X ray fluorescence, Molecular orbitals, X rays, Reprints, \*Chlorotrifluoromethane, \*Trichloro-

A new technique sensitive to molecular orientation and geometry, and based on measuring the polarization of x-ray emission, has been applied to the Cl-containing molecules methyl chloride (CH3Cl) and the chlorofluoromethanes (CF3Cl, CF2Cl2, and CFCl3) in the gas phase. Upon selective excitation using monochromatic synchrotron radiation in the CI K-edge (CI 1s) near-threshold region, polarization-selective x-ray emission studies reveal highly polarized molecular valence x-ray fluorescence for all four molecules. It is shown that the polarized x-ray emission technique can be used to infer, directly from experiment, symmetries of occupied and unoccupied valence molecular orbitals, anisotropies in absorption and emission, and ori-entational and geometrical information. It is suggested that the x-ray polarized-fluorescence phenomenon, reported here for simple molecules, can be used as a new approach to study more complicated systems in a variety of environments.

100.330

PB91-175059 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Chemical Kinetics Div.

Group Reactivities in the Gas Phase Reactions of Hydroxyl Radicals with Ethers.

Final rept. R. Liu, T. J. Wallington, P. Dagaut, and M. J. Kuryio. 1989, 4p

Pub. in Wuli Huaxue Xuebao 5, n2 p210-213 1989.

Keywords: \*Hydroxy radicals, \*Ethers, \*Reaction kinetics, Chemical reactivity, Photolysis, Reprints, Chemical functional groups, Gas phase.

The absolute rate constant was determined for the gas phase reaction of OH radicals with diethoxy methane using the flash photolysis resonance fluorescence technique. OH + CH3CH2OCH2OCH2CH3 -> products (1) Experiments were performed at total pressures (using Ar diluent gas) between 25-50 torr. The authors' earlier kinetic measurements for normal ali-phatic mono-ethers are used to calculate reactivity values for CH3 and CH2 which are significantly enhanced over those in normal alkanes. These values predioct the rate constant for reaction (1) quite accurately, indicating that there is no further reactivity enhancement due to the second functional group.

100.331

PB91-175133 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Chemical Kinetics Div.

Single Pulse Shock Tube Study of the Reactions of Hydrogen Atoms with Aromatics. 4. Chlorotoluenes.

Final rept.

W. Tsang, Y. Z. He, W. G. Mallard, and J. P. Cui. 1988, 8p

Pub. in Shock Tubes and Waves, p467-474 1988.

Keywords: \*Hydrogen, \*Atoms, \*Reaction kinetics, Displacement reactions, Thermodynamics, Shock tubes, Reprints, \*Chlorotoluenes, Hydrogen atom abstraction.

The hydrogen atom induced decomposition of para and ortho chlorotoluene was studied in single pulse shock tube experiments. The hydrogen atoms are generated through the decomposition of trace quantities of hexamethylethane in large excesses of the chlorotoluene. The displacement products, chlorobenzene and toluene, are directly detected. The importance of the abstraction channel is determined by the difference between the total amount of isobutene, produced in equal molar quantities with the H-atoms, and the dis-placement products. With rate constants for hydrogen atom attack on methane as internal standards, the rate expressions for the three parachlorotoluene decompoexplessions of the three parachiotototeric decomposition channels have been found to be,  $k(H+p-ClC6H4CH3-H2+ClC6H4CH2)=9.6\times10$  to the 10th power Exp(-4265/T) |/mol-s k(H+p-ClC6H4CH3-CH+ClC6H5)=3.5 × 10 to the 10th power Exp(-3710/T) |/mols k(H+p-ClC6H4CH3-Cl3+C6H4CH3)=4.8 × 10 to the tenth power Exp(-4795/T) |/mol-s at 1010 - 1130. The measurments for orthoclorotoluene are more difficult due to the presence of toluene and chlorotoluene impurities. The rate constants for the comparable processes are close to that for the parachloro compound and have been found to be factors of 1.2,1.3, and 1.1 of the values given above. The authors results are compared with previously published numbers of toluene and phenol.

PB91-175174 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Molecular Spectroscopy Div.

Molecular Spectroscopy Division of the National

Bureau of Standards.

Final rept.

A. Weber. 1987, 2p
Pub. in Applied Spectroscopy 41, n6 p1085-1086

Keywords: \*Molecular spectroscopy, US NBS, Reseárch, Reprints.

The report is a brief description of the activities of the Molecular Spectroscopy Division at the National Bureau of Standards. 100.333

PB91-175257 Not available NTIS National Bureau of Standards (NEL), Boulder, CO. Chemical Engineering Science Div.

Book Review: Partitioning in Aqueous Two-Phase Systems: Theory, Methods, Uses, and Applications to Biotechnology.

Final rept.

G. F. Slaff. 1987, 1p Pub. in Jnl. of American Chemical Society 109, n5 p1606 1987.

Keywords: \*Phase, \*Partition, Solvent extraction, Separation, Reviews, Biotechnology, Reprints, \*Aqueous systems

This is a review of the book, 'Partitioning in Aqueous Two-Phase Systems'.

100.334

PB91-175505 Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Quantum Physics Div.

Rotational Predissociation, Vibrational Mixing, and van der Waals Intermolecular Potentials of NeDF. Final rept.

C. M. Lovejoy, and D. J. Nesbitt. 1991, 16p Grant NSF-CHE86-05970

Sponsored by National Science Foundation, Washington, DC.

Pub. in Jnl. of Chemical Physics 94, n1 p208-223, 1 Jan 91.

Keywords: \*Neon complexes, Van der Waals forces, Hydrogen fluoride, Deuterium compounds, Supersonic jet flow, Infrared spectroscopy, Laser spectroscopy, Binding energy, Near infrared radiation, Predissocia-tion, Neon 20, Neon 22, Potentials, Reprints.

The near-infrared spectrum of NeDF formed in a slit free jet expansion is recorded with a high resolution, tunable laser spectrometer. Four bands, consisting of the DF stretching fundamental and three internal rotation and van der Waals stretch combination bands, are observed and analyzed for both the 20Ne and 22Ne isotopomers. All three combination bands reveal a sudden onset of rotational predissociation at modest J, which is modeled with effective one-dimensional potentials to determine the binding energy. The experi-mental results are compared with predictions of a recently published ab initio anisotropic potential surface, and an improved potential is developed and tested.

100,335

PB91-175562 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Quantum Metrology Div.

Direct Determination of Molecular Orbital Symmetry of H2S Using Polarized X-ray Emission. Final rept.

R. Mayer, D. W. Lindle, S. H. Southworth, and P. L. Cowan. 1991, 7p

Pub. in Physical Review A 43, n1 p235-241, 1 Jan 91.

Keywords: \*Hydrogen sulfide, \*Molecular orbitals, Polarization(Waves), Emission spectra, X rays, Symmetry, Reprints.

X-ray emission from the molecule H2S is strongly polarized following excitation of a sulfur K-shell electron to an unoccupied subthreshold molecular orbital with a polarized x-ray beam. Changes in the polarization of the emission spectrum are observed as the incident beam's energy is swept across the subthreshold absorption resonance. The previously unresolved absorption resonance is shown experimentally to be primarily associated with a molecular orbital of b2 symmetry, but with a high-excitation-energy component due to an orbital with a1 symmetry. Satellite emission intensity is shown to depend on the primary photon energy, and is therefore associated with multivacancy effects and not with contamination, as previously sugaested.

100.336

PR91-187138 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Center for Chemical Physics.

# **Physical & Theoretical Chemistry**

Concerning the Formation and the Kinetics of Phenylium lons.

Final rept. P. Ausloos, S. G. Lias, T. J. Buckley, and E. E. Rogers. 1989, 13p
Pub. in International Jnl. Mass Spectrom. Ion Process-

es 92, p65-77 1989.

Keywords: \*Reaction kinetics, Organic ions, Isomerization, Hydrocarbons, Molecular structure, Potential energy, Reprints, \*Phenylium ions, Ion molecule reactions, Halobenzenes, Pulsed ion cyclotron spectrome-

Kinetic measurements carried out in a pulsed ion cyclotron spectrometer show that C6H5(+) ions formed in unimolecular and bimolecular processes can exhibit two populations of different reactivities. As expected, ground-state singlet phenylium ions are predominantly formed in low energy processes, while higher energy isomeric (mainly acyclic) ions appear in the high energy electron impact fragmentation of C6H6 and halobenzenes, as well as in highly exothermic ion/mole-cule reactions. The energy barrier for ring opening was estimated to be 2.0 + or - 0.3 eV, in reasonably good agreement with theory. Phenylium ions react readily with hydrocarbons and polar molecules. By means of isotopic labelling it was shown that alkanes transfer H2 via a two-stage process consisting of the transfer of  $H(\cdot)$  to the phenylium ion followed by a transfer in the complex of H(+) to the resulting benzene moiety. Cyclopropane was found to transfer CH2 to the phenylium ion in a direct concerted process. In contrast, reaction with unsaturated hydrocarbons involves extensive hydrogen and carbon atom scrambling. Contrary to earlier findings phenylium ions were found to react at least ten times faster with acetylene than the other C6H5(+) isomer(s).

Not available NTIS
National Bureau of Standards (NEL), Gaithersburg,
MD. Thermodynamics Div.
Critical Exponent for the time.

Liquids.

Final rept.

R. F. Berg, and M. R. Moldover. 1988, 11p Contract NASA-C-86129D Sponsored by National Aeronautics and Space Administration, Cleveland, OH. Lewis Research Center. Pub. in Jnl. of Chemical Physics 89, n6 p3694-3704

Keywords: \*Viscosity, \*Binary mixtures, \*Liquids, Viscometry, Viscoelasticity, Critical temperature, Re-

We have measured the viscosity of four binary mixtures near their consolute points: (1) methanol + cyclohexane, (2) isobutyric acid + water, (3) nitroethane + 3-methylpentane, and (4) 2-butoxyethanol + water. The viscosity data are consistent with the power-law divergence: eta approximately equal to (T-Tc)(-y), with an apparent viscosity exponent in the range 0.0404 < 0.0444. Recent theoretical estimates for y are near 0.032, which is outside the experimental range. The value of y is independent of whether the critical point is an upper or a lower consolute point and of whether the approach toward Tc is at constant pressure or at constant volume. Our torsion oscillator viscometer is unique in its simultaneous low frequency (1 Hz) and low shear rate (0.1/s), allowing its use close to the critical point before encountering non-Newtonian fluid behavior associated with critical slowing down. Nevertheless, we find quantitative evidence for viscoelasticity near the critical point.

PB91-187435 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Radiometric Physics Div. Shape Resonances in Molecular Fields.

Final rept.

J. L. Dehmer, D. Dill, and A. C. Parr. 1988, 23p See also DE84009206.

Pub. in Fundamental Processes of Atomic Dynamics, p541-563 1988.

Keywords: Electron-molecule collisions, Electron scattering, Photoionization, Molecular models, Spectroscopy, Nitrogen, Reprints, \*Shape resonances.

A shape resonance is a quasibound state in which a particle is temporarily trapped by a potential barrier (i.e., the shape of the potential), through which it may eventually tunnel and escape. This simple mechanism plays a prominent role in a variety of excitation processes in molecules, ranging from vibrational excitation by slow electrons to ionization of deep core levels by xrays. Moreover, their localized nature makes shape re-sonances a unifying link between otherwise dissimilar circumstances. One example is the close connection between shape resonances in electron-molecule scattering and in molecular photoionization. Another is the frequent persistence of free-molecule shape resonant behavior upon adsorption on a surface or condensa-tion into a molecular solid. The main focus of the arti-cle is a discussion of the basic properties of shape re-sonances in molecular fields, illustrated by the sigma(sub u) shape resonance in N2. Other aspects to be discussed are vibrational effects of shape resonances, connections between shape resonances in different physical settings, and examples of shape resonant behavior in more complex cases, which form current challenges in the field.

100,339 PB91-187658

(Order as PB91-187617, PC A06/MF A01) National Inst. of Standards and Technology, Gaithers-

Durg, MD.
Proposed New Electrolytic Conductivity Primary Standards for KCI Solutions.
Y. C. Wu, W. F. Koch, and K. W. Pratt. 1991, 11p Included in Jnl. of Research of the National Institute of Standards and Technology, v96 n2 p191-201 Mar/Apr

Keywords: \*Primary standards, \*Aqueous electrolytes, \*Potassium chloride, \*Standards, Electrical conductivity, \*Electrolytic conductivity, Cell constants, Demal.

An absolute determination of aqueous electrolytic conductivity has been made for 0.01 molal (m) and 0.1 m potassium chloride solutions, over the temperature range of 0 to 50 C in 5 degree intervals. A cell with a removable center section of accurately known length and area was used for the measurements. Values were adjusted to be in conformity with the ITS-90 temwere adjusted to be in conformity with the 113-90 temperature scale. The overall uncertainty over the entire temperature range is estimated to be 0.03%. Values at 25 C for 0.01 and 0.1 m are 0.00140823 and 0.0128246 S/cm, respectively. It is proposed that these values be adopted as primary standards for aqueous electrolytic conductivity, replacing the demal

100,340 PB91-189233 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Chemical Thermodynamics Div. Combustion Calorimeters. Final rept.

Pub. in Advances in Calorimetry and Thermochemistry, v1 p51-111 1990.

Keywords: \*Heat measurement, \*Combustion, \*Calorimetry, Physical chemistry, Thermodynamics, Reviews, Thermochemistry, US NBS, Reprints.

The paper provides a survey of ongoing activities in combustion calorimetry in the Chemical Thermodynamics Division at the National Bureau of Standards (NBS), USA. For some time, many physical chemists have felt that the frontiers of combustion calorimetry have disappeared and that little novelty or innovation is required for the application of the technique. Moreover, they also felt that the impact of new develop-ments in the area of physical chemistry would not be very significant. The paper seeks to demonstrate that significant innovation in combustion calorimetric methods is occurring, and that significant accomplishments have been made and should be expected for the future in the area of research.

100,341 PB91-189241 Not available NTIS National Inst. of Standards and Technology (IMSE), Gaithersburg, MD. Polymers Div. How Does Surface Roughness Affect Polymer-Surface Interactions.

Final rept. 7. F. Douglas. 1989, 10p Pub. in Macromolecules 22, n9 p3707-3716 Sep 89.

Keywords: \*Surface roughness, \*Fractals, \*Adsorption, \*Fluid-solid interactions, \*Polymers, Liquid-solid interfaces, Entropy, Mathematical models, Monte Carlo Method, Invariance, Reprints.

A simple model is introduced to qualitatively describe the effect of surface roughness on the propertiies of surface interacting polymers and comparison is made with recent Monte Carlo data and renormalization group calculations. The model indicates that increasing the surface irregularity (i.e. the fractal dimension) has the effect of enhancing polymer-surface interac-tions relative to the idealized planar interface. This is a consequence of a greater probability of polymer-sur-face intersection with increasing roughness. It is also argued that adsorption occurs more readily on fractal surfaces since then adsorption requires a smaller 'entropic price'. A rough surface (fractal dimension = 3) may adsorb a polymer when a corresponding smooth surface (fractal dimension = 2) of the same material will not adsorb. Roughness can thus alter the effective polymer-surface interaction in a fundamental way.

100,342 PB91-189381 PB91-189381 Not available NTIS National Bureau of Standards (NEL), Gaithersburg,

MD. Thermophysics Div.

Modeling the Thermodynamic Properties of Sodium Chloride in Steam Through Extended Corresponding States.

Final rept. J. S. Gallagher, and J. M. H. Levelt Sengers. 1988,

Pub. in International Jnl. of Thermophysics 9, n5 p649-661 1988.

Keywords: \*Sodium chloride, \*Solutions, \*Thermodynamic properties, \*Phase transformations, Aqueous electrolytes, Steam, Helmboltz free energy, Critical pressure, Critical temperature, Mathematical models, Reprints, \*Apparent molar specific heat, \*Apparent molar volume, Corresponding states.

Recent precise data on anomalous behavior of apparent molar properties of electrolyte solutions in nearcritical steam have raised important questions as to how the thermodynamic properties of these systems should be described. Current Gibbs free energy models fail for highly compressible solutions. Here, a Helmholtz free energy formulation is presented as a first step in modelling compressible dilute aqueous electrolyte solutions. Comparisons are made with the known critical line, coexistence curves, apparent molar volumes and specific heats of NaCl in steam, and conclusions presented on improving the model.

PB91-189415 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Molecular Spectroscopy Div.

Spectroscopic Constants for the nu9 Infrared Band of HNO3. Final rept.

A. Goldman, A. G. Maki, C. J. Howard, J. B. Burkholder, and R. Escribano. 1988, 6p Pub. in Jnl. of Molecular Spectroscopy 131, n1 p195-200 1988

Keywords: \*Nitric acid, \*Spectrum analysis, \*Infrared spectroscopy, Vibrational spectra, Rotational spectra, Atmospheric chemistry, Air pollution, Reprints.

High resolution infrared measurements have been made on the nu 9 band of HNO3 from 414 to 500/cm. Over 2300 transitions have been measured, assigned, and fit to obtain 14 ro-vibrational constants for the nu9=1 state that reproduce the observed spectrum with a RMS deviation of 0.0004/cm. The band center for nu 9 is at 458.2887 + or - 0.0005/cm.

Not available NTIS PB91-189431 National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Thermophysics Div.

Effect of Long Range Interfacial Forces on the Dynamics of Wetting Layers at a Liquid Vapor Inter-

Final rept. J. L. Harden, and R. F. Kayser. 1989, 10p Pub. in Jnl. of Colloid and Interface Science 127, n2 p548-557 1989.

Keywords: \*Liquid-vapor interfaces, Van der Waals forces, Light scattering, Capillary waves, Thickness, Wetting, Reprints.

For certain binary liquid solutions, the denser fluid will form a thin wetting layer between the less dense fluid and the vapor. The authors consider the possible effect of interfacial van der Waals forces on the capillary waves residing on such wetting layers. In the limit where wetting layer thickness, h, is much smaller than

the capillary wavelength, they find a damped peristaltic mode that behaves as (omega squared) varies as (k squared)/(h cubed) for typical wave numbers. Such a mode, if observable, could provide an alternate means of measuring wetting layer thicknesses and could be used to check the dependence of wetting layer thickness on long range interfacial forces.

100,345 PB91-189514 Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Thermophysics Div.

Mobility Fluctuations and Electrophoretic Light

Scattering from Macromolecular Solutions. Final rept.

J. B. Hubbard, and D. A. McQuarrie. 1988, 15p Pub. in Jnl. of Statistical Physics 52, n5-6 p1247-1261 1988

Keywords: \*Macromolecules, Light scattering, Sto-chastic processes, Electrophoresis, Solutions, Mobility, Reprints.

The authors discuss the origins and the effects of mobility fluctuations of rigid, globular macromolecules on a solution's electrophoretic light scattering spectrum. Assuming a dilute solution, a modified van Hove self-correlation function is calculated via van Kampen's time-ordered cumulant method, and the results are compared with less rigorous approaches. The consequences of generalizing to dynamic external fields are briefly considered.

100.346 PB91-189548 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Chemical Kinetics Div.

Electronic Spectrum of the GeH3 Radical.

R. D. Johnson, J. W. Hudgens, and B. P. Tsai. 1988, 6p Pub. in Jnl. of Chemical Physics 89, n8 p4558-4563 1988.

Keywords: Free radicals, Rydberg states, Vibrational states, Chemical reactions, Chlorine, Fluorine, Reprints, \*Germyl radicals, Multiphoton ionization.

The germyl (GeH3) radical has been observed by resonance enhanced multiphoton ionization (REPI) spectroscopy in the region of 370 - 430 nm. The spectrum arises from two-photon resonances with the 5p doublet A double prime, sub 2 (D sub 3h) Rydberg state that possesses an origin at 419.1 nm (v0-0)=47,705/cm). A vibrational progression of 758/cm was assigned to the 'umbrella' mode, v' sub 2. The observed X doublet A sub 1 (C sub 3V) (V double prime, sub 2) = 2 to (V double prime, sub 2) = 0 vibrational interval is 663/cm which leads to an estimated barrier to inversion of 1530/cm.

100.347

PB91-189613 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Chemical Thermodynamics Div. Energy of Combustion of Triphenylphosphate. Final rept.

D. R. Kirklin, and E. S. Domalski. 1989, 8p Pub. in Jnl. of Chemical Thermodynamics 21, n5 p449-456 1989

Keywords: \*Heat of combustion, \*Heat of formation, Phosphorus organic acid esters, Heat measurement, Heatof fusion, Heat of vaporization, Reprints, \*Triphonylphosphate.

The enthalpy of combustion of crystalline triphenyl-phosphate was measured in the NBS aneroid adiabatphosphate was measured in the NBS aneroid adiabatic rotating calorimeter. The standard molar enthalpy of combustion at 298.15 K and 1 bar P(o)=100,000Pa for the reaction: C18H15PO4(cr) + 21 O2(g) = 18 CO2(g) + (H3PO4 + 6 H2O)(aq) is-(9259.31 + or -4.96) kJ/mol. The derived enthalpy of formation for crystalline triphenylphosphate is -(829.26 + or - 5.72) kJ/mol. Enthalpies of formation of the liquid and gas phases were calculated using literature values of the enthalpies of fusion and vaporization. Group contribution values were derived for estimating enthalpies of formation of aromatic phosphates in the gas, liquid, and solid phases.

PB91-189639 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Molecular Spectroscopy Div.

Hydrogen Bonding in Pt Ammine Complexes.

Final rept. M. Krauss, K. J. Miller, and H. Basch. 1988, 4p Pub. in Chemical Physics Letters 148, n6 p577-580 1988

Keywords: \*Platinum complexes, \*Ammino compounds, \*Bonding strength, \*Hydrogen bonds, Oligon-ucleotides, Mathematical models, Calculation meth-ods, Guanines, Formaldehyde, Carbonyl compounds,

Intra- and inter-ligand hydrogen bonding stabilize the binding of Pt ammine complexes to oligonucleotides. Model calculations explore the energetics of intraligand binding of the ammine to G(06) in PtA3G (A=ammine, G=guanine) and the inter-ligand binding of a carbonyl oxygen to the ammine in a complex of PtA4 and formaldehyde. Hydrogen bonding interaction to the G(06) site yields a weak bonding interaction but permits the close approach of the guanine(06) and ammine(H) atoms. Inter-ligand hydrogen bonding is strong as expected for an optimal ionic hydrogen

PB91-189837 Not available NTIS National Bureau of Standards (NEL), Gaithersburg,

MD. Thermophysics Div.

Modelling Aqueous Solutions Near the Critical

Point of Water.

Final rept. G. Morrison. 1988, 21p Pub. in Jnl. of Solution Chemistry 17, n9 p887-907 1988

Keywords: \*Aqueous electrolytes, \*Solutions, \*Thermodynamic properties, \*Partial molar volume, Water, Dilution, Critical temperature, Critical pressure, Helmholtz free energy, Mathematical models, Reprints, \*Nonelectrolytes, \*Partial molar isobaric thermal expansion.

The thermodynamic properties of a dilute solution near the critical point of the solvent are discussed. Two ex-amples are discussed, a solution of a nonelectrolyte and a solution of an electrolyte. The limiting behavior of the electrolyte solutions is modelled with a Debye-Huckel term in the Helmholtz free energy. The partial molar properties, in particular the volume and isobaric thermal expansion are examined in detail. The derivation of these properties is introduced by considering the geometry of the thermodynamic surfaces near to and far from the critical point of the solvent. The authors conclude that the properties of solutions near the solvent critical point are dominated by that feature; solution properties cannot be adequately modelled without including the functional forms associated with the critical point.

100,350 PB91-189845 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Thermophysics Div.

Ergodic Measures for the Simulation of Dielectric

Properties of Water.

Final rept. R. D. Mountain, and D. Thirumalai. 1991, 8p Sponsored by National Science Foundation, Washing-

ton, DC.
Pub. in Computer Physics Communications 62, p352-359 1991

Keywords: \*Water, Dielectric properties, Time intervals, Dipole moments, Computerized simulation, Hydrogen bonds, Reprints, Molecular dynamics.

The authors determine the time interval t(obs), required for effective ergodic convergence of the fluctuations in dipole moment which are needed for the computation of the dielectric properties of water. It is established that the value of t(obs) can be computed from the scaling relations obeyed by the fluctuation metric, Omega sub mu (t), associated with the time-averaged values of the dipole moment of the individual water molecules. The theoretical ideas behind Omega sub mu (t) are used to compute t(obs) at several temperatures for the simple point-charge model of water. It is found that t(obs) increases exponentially with decreasing temperature, the barrier being associated with the difficulty in making collective orientational rearrangements. For the simple point-charge model considered in the paper, the barrier for these collective motions is estimated to be 3.5 kcal/mole. The study provides a firm basis for obtaining reliable values of the dielectric properties of dipolar fluids using molecular dynamics simulations.

100.351 PB91-189852 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Chemical Kinetics Div.

Polyelectrolyte Stabilized Metal Oxide Hydrosols as Catalysts for the Photooxidation of Water by Zinc Porphyrins.

Final rept. G. S. Nahor, S. Mosseri, P. Neta, and A. Harriman. 1988, 6p

Pub. in Jnl. of Physical Chemistry 92, n15 p4499-4504

Keywords: \*Iridium oxides, \*Ruthenium oxides, \*Catalysts, \*Water, \*Hydrosols, \*Photooxidation, Porphyrins, Quantum efficiency, Oxygen, Solar energy, Reaction kinetics, Reprints.

Colloids of ruthenium dioxide and iridium oxide have been prepared and characterized. These colloids, which are inherently negatively-charged in neutral water, have been stabilized with a surface layer of polyelectrolyte. Electrostatic binding occurs between the stabilized colloids and water-soluble zinc porphyrins of the opposite electronic charge. Such electrostatic forces affect the rate constant for interfacial electron transfer between the colloids and radical cations derived from the zinc porphyrins. The products of these reactions depend upon the relative charges of the reactants. For oppositely charged reactants, the rate of interaction was very high but O2 generation was not observed. In cases where the porphyrin and colloid possess the same charge, the system can be used to oxidize water to O2 under photochemical conditions. The yield of O2 depends upon the solution pH and the nature of both reactants. With negatively charged reactants in alkaline solution, the authors have reported quantum efficiencies for O2 generation in the range of 50-60%. With positively charged reactants, oxygen formation could be observed in acidic solution, although the quantum efficiencies were less than 10%.

100 352

PB91-189902 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Chemical Kinetics Div.

Proton Affinity of Cyanogen and Ion-Molecule Reactions of C2N2(+).

Final rept.

S. A. H. Petrie, M. Mautner, M. J. McEwan, and C. G.

Freeman. 1989, 10p Pub. in International Jnl. of Mass Spectrometry and Ion Processes 90, n3 p241-250 1989.

Keywords: \*Cyanogen, Nitriles, Reaction kinetics, Thermochemistry, Thermodynamics, Organic ions, Hydrocarbons, Carbon monoxide, Carbon dioxide, Reprints, \*Proton affinity, \*Ion molecule reactions

The proton affinity (PA) of C2N2 has been determined by proton transfer equilibria using forward and reverse rate coefficients from SIFT measurements. The results yield a PA for CH3Cl of 673 + or - 4 kJ/mol and a PA for C2N2 of 674 + or - 4 kJ/mol relative to a PA for C2H4 of 680 + or - 2 kJ/mol. C2N2H + is also formed by the reactions of C2N2(+) with H2 and H2O. In the latter, charge transfer competes with H atom transfer, while in the reaction of C2N2(+) with C2H2 and C2H4, only charge transfer occurs. In each instance for these reactions of C2N2(+), the most exothermic channel is dominant and occurs at or near the collision rate. Rate coefficients are also reported for association (condensation) of C2N2(+) with CO, CO2, C2H2 and C2H4.

100,353 Not available NTIS PB91-189936 National Inst. of Standards and Technology (NML), Gaithersburg, MD. Surface Science Div.

Recent Developments in Applied Surface Science. Final rept.

C. J. Powell. 1989, 2p Pub. in Vide, Couches Minces 44, n248 p427-428

Keywords: \*Surfaces, Reprints, Overviews.

An overview is given of the recent growth of applied surface science and of the recent proposal to form an Applied Surface Science Division within the International Union of Vacuum Science, Technique and Applications

100.354

PB91-192435

Not available NTIS

# **Physical & Theoretical Chemistry**

American Chemical Society, Washington, DC. Journal of Physical and Chemical Reference Data, Volume 19, Number 4, July-August 1990. Bimonthly rept.

D. R. Lide. c1990, 270p See also PB91-192443 through PB91-192468 and PB90-244658. Errata sheet inserted. Prepared in cooperation with American Inst. of Physics, New York. Sponsored by National Inst. of Standards and Technology, Gaithersburg, MD.
Available from American Chemical Society, 1155 16th St., NW, Washington, DC. 20036-9976.

Keywords: \*Sulfur, \*Atomic energy levels, \*Atomic spectra, \*Specific heat, \*Entropy, \*Solids, Phase transformations, Sulfur ions, Thermodynamic properties, Enzymes, \*Liquids, \*Krebs Cycle, \*Organic acids, \*Amino acids, \*Organic compounds, Oxidation reduction reactions. tion reactions.

Energy Levels of Sulfur, S(I) Through S(XVI); Heat Capacities and Entropies of Organic Compounds in the Condensed Phase, Volume

II; The Thermodynamics of the Krebs Cycle and Related Compounds.

Not available NTIS PB91-192443 National Inst. of Standards and Technology (NML), Gaithersburg, MD. Center for Atomic, Molecular and Optical Physics.

Energy Levels of Sulfur, S I Through S XVI. Bimonthly rept.

W. C. Martin, R. Zalubas, and A. Musgrove. c1990, 60p

Included in Jnl. of Physical and Chemical Reference Data, v19 n4 p821-880 Jul/Aug 90. Available from American Chemical Society, 1155 16th St., NW, Washington, DC. 20036-9976.

Keywords: \*Sulfur, \*Atomic energy levels, \*Atomic spectra, Sulfur ions, Ionization potentials, Electron configurations.

Energy level data are given for the atom and all positive ions of sulfur (Z = 16). These data have been critically compiled, mainly from published and unpublished material on measurements and analyses of the optical spectra. The authors have derived or recalculated the levels for a number of the ions. In addition to the level values in reciprocal cm and the parity, the J value and the configuration and term assignments are listed if known. Leading percentages from the calculated eigenvectors are tabulated or quoted wherever available. Ionization energies are given for all spectra.

Not available NTIS PB91-192450 National Inst. of Standards and Technology (NML), Gaithersburg, MD. Chemical Thermodynamics Div. Heat Capacities and Entropies of Organic Compounds in the Condensed Phase. Volume 2.

Bimonthly rept.
E. S. Domalski, and E. D. Hearing. c1990, 168p
Included in Jnl. of Physical and Chemical Reference
Data, v19 n4 p881-1048 Jul/Aug 90. Available from
American Chemical Society, 1155 16th St., NW, Wash ington, DC. 20036-9976.

Keywords: \*Specific heat, \*Entropy, \*Liquids, \*Solids, \*Organic compounds, Tables(Data), Reviews, Thermodynamic properties, Phase transformations.

The compilation of data on the heat capacities, entropies, and phase transitions of organic compounds in the condensed phase supplements the document pubthe condensed phase supplements the document published earlier on the subject, namely 'Heat Capacities and Entropies of Organic Compounds in the Condensed Phase' by E. S. Domalski, W. H. Evans, and D. Hearing, J. Phys. Chem. Ref. Data, 13, Suppl. 1, (1984). It provides data on approximately 1300 organic compounds. About half of the articles examined contain data published prior to 1982. A total of 565 articles have been examined, evaluated, and referenced. In addition to values for the heat capacity and entropy at 298.15 K, phase transitions for solid/solid, solid/liquid, and in some instances, solid/gas and liquid/gas are tabulated as encountered from the articles examined and evaluated.

100,357 PB91-192468 Not available NTIS California Univ., San Diego, La Jolla. Dept. of ChemisThermodynamics of the Krebs Cycle and Related Compounds.

Bimonthly rept. S. L. Miller, and D. Smith-Magowan. c1990, 25p Grant NANB6-D0656

Prepared in cooperation with National Inst. of Standards and Technology (NML), Gaithersburg, MD. Chem-

ical Thermodynamics Div.
Included in Jnl. of Physical and Chemical Reference
Data, v19 n4 p1049-1074 Jul/Aug 90. Available from
American Chemical Society, 1155 16th St., NW, Washington, DC. 20036-9976.

Keywords: \*Krebs Cycle, \*Entropy, \*Heat of formation, \*Gibbs free energy, \*Aspartic acid, \*Citric acid, \*Acetic acid, \*Furmaric acid, \*Formic acid, \*Glutamic acid, \*Succinic acid, \*Organic acids, \*Alanines, \*Glycine, Chemical equilibrium, Metabolism, Enzymes, Catalysis, Oxidation reduction reactions.

A survey is made of the enthalpies of formation, third law entropies and Gibbs energies available for Krebs cycle and related compounds. These include formate, acetate, succinate, fumarate, glycine, alanine, aspartate and glutamate. The potential of the NAD+/NADH couple is recalculated based on the ethanol/acetaldehyde and isopropanol/acetone equilibria. The reported enzyme catalyzed equilibrium constants of the Krebs cycle reactions are evaluated with estimated errors.

These 28 equilibria form a network of reactions that is solved by a least squares regression procedure giving Gibbs energies of formation for 21 Krebs cycle and related compounds. They appear to be accurate to + or -0.4 kJ/mol for some compounds but + or -1 kJ/mol in less favorable cases. This procedure indicates which third law delta(sub f) and enzyme equilibria are inaccurate, and allows very accurate delta(sub f) to be determined for compounds related to the Krebs cycle by measuring enzyme equilibrium constants.

PB91-192476 Not available NTIS American Chemical Society, Washington, DC.
Journal of Physical and Chemical Reference Data,
Volume 19, Number 5, September-October 1990. Bimonthly rept.

D. R. Lide. c1990, 202p See also PB91-192484 through PB**9**1-192534. Prepared in cooperation with American Inst. of Physics, New York. Sponsored by National Inst. of Standards and Technology, Gaithersburg, MD.

Available from American Chemical Society, 1155 16th

St., NW, Washington, DC. 20036-9976.

Keywords: \*Thermodynamic properties, Liquid oxygen, Polyatomic gases, Thermal conductivity, Carbon tetrafluoride, Methane, Molten salts, Phase diagrams, Rare gases, Water.

Transport Properties of Fluid Oxygen; Thermal Conductivity of Nine Polyatomic Gases

at Low Density;
The Thermal Conductivity of Methane and
Tetrafluoromethane in the Limit of Zero

Density;
Coupled Phase Diagram-Thermodynamic Analysis of the 24 Binary Systems, A2CO3-AX and A2SO4-AX Where A = Li, Na, K and X = Cl, F, NO3, OH;

Equilibrium and Transport Properties of Gas Mixtures at Low Density--Eleven Polyatomic

Gases and Five Noble Gases; A Unified Fundamental Equation of State for the Thermodynamic Properties of H2O.

PB91-192484 Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Thermophysics Div. Not available NTIS Transport Properties of Fluid Oxygen.

Bimonthly rept. A. Laesecke, R. Krauss, K. Stephan, and W. Wagner. c1990, 34p

Prepared in cooperation with Stuttgart Univ. (Germany, F.R.). Inst. fuer Technische Thermodynamik und Thermische Verfahrenstechnik, and Ruhr Univ., Bochum (Germany, F.R.). Inst. fuer Thermo- und Fluiddynamik. Included in Jnl. of Physical and Chemical Reference Data, v19 n5 p1089-1122 Sep/Oct 90. Available from American Chemical Society, 1155 16th St., NW, Washington, DC. 20036-9976.

Keywords: \*Liquid oxygen, \*Oxygen, Transport properties, Thermal conductivity, Viscosity, Equations of state, Graphs(Charts).

Supplementing the recently completed IUPAC tables for the thermodynamic properties of oxygen, the paper presents a data evaluation of the transport properties, viscosity, and thermal conductivity. From a comprehensive literature survey the available data have been compiled, and their quality was assessed. Selected measurements were correlated to generate skeleton tables of the most reliable data along the vapor-liquid coexistence curve and for the fluid region at pressures from 0.1 to 100 MPa and at temperatures from 70 to 1400 K. The set of correlations which was developed includes residual concept formulations as well as transport equations of state. These allow the direct calculation of viscosities and thermal conductivities from pressure and temperature as input variables. The simplified crossover model was employed to represent the enhancement of the thermal conductivity in the critical region.

100.360

Not available NTIS PB91-192492 Universidad Autonoma Metropolitana, Mexico City. Dept. of Fisica.

Thermal Conductivity of Nine Polyatomic Gases at Low Density.

Bimonthly rept.
F. J. Uribe, E. A. Mason, and J. Kestin. c1990, 14p
Grants NSF-CHE85-09416, NSF-CHE88-19370
Prepared in cooperation with Brown Univ., Providence,

RI. Sponsored by National Science Foundation, Washington, DC., and National Inst. of Standards and Technology, Gaithersburg, MD.
Included in Jnl. of Physical and Chemical Reference Data, v19 n5 p1123-1136 Sep/Oct 90. Available from American Chemical Society, 1155 16th St., NW, Washington DC. 20036-9076

ington, DC. 20036-9976.

Keywords: \*Polyatomic gases, \*Thermal conductivity, Nitrogen, Oxygen, Nitrogen oxide(NO), Nitrogen oxide(N2O), Carbon monoxide, Carbon dioxide, Carbon tetrafluoride, Sulfur hexafluoride, Methane, Tables(Data).

The authors present a complete set of easily programmable computer algorithms, and a set of numerical tables, for the thermal conductivities of the nine gases: N2, O2, NO, CO, CO2, N2O, CH4, CF4, and SF6. This complements their earlier corresponding-states work on the equilibrium and transport properties of these gases (J. Phys. Chem. Ref. Data 16, 445 (1987); 17, 255 (1988)). The results embrace the temperature range from T star = kT/epsilon = 1 up to a nominal upper limit of 3000 K. The accuracy achieved is specific fied, and the correlation can be used in a predictive mode.

100,361

PB91-192500 Not available NTIS Imperial Coll. of Science and Technology, London (England). Dept. of Chemical Engineering and Chemical Technology.

Thermal Conductivity of Methane and Tetrafluoromethane in the Limit of Zero Density.

Bimonthly rept. M. J. Assael, J. Millat, V. Vesovic, and W. A.

M. J. Assael, J. Millat, v. vesovic, and w. A. Wakeham. c1990, 11p Sponsored by National Inst. of Standards and Technology, Gaithersburg, MD., Department of Industry. London (England), and Rostock Univ. (German D.R.). Included in Jnl. of Physical and Chemical Reference Data, v19 n5 p1137-1148 Sep/Oct 90. Available from American Chemical Society 1155 16th St. NW Wash-American Chemical Society, 1155 16th St., NW, Washington, DC. 20036-9976.

Keywords: \*Carbon tetrafluoride, \*Methane, \*Thermal conductivity, Polyatomic gases, Transport properties, Tables(Data).

The paper presents accurate representations of the thermal conductivity of methane and tetrafluoromeththermal conductivity of methane and tetrafluoromethane in the limit of zero density. The theoretically-based correlations provided are valid for the temperature range 120-1000 K and 280-750 K for methane and tetrafluoromethane respectively. The methane correlation has associated uncertainties of + or - 2% between 300 and 500 K, rising to + or - 2.5% at the low, and + or - 4% at the high, temperature extremes. The tetrafluoromethane correlation has uncertainties of 1% between 280 K and 450 K, rising to + or - 5% at the highest temperature. A comparison with some earlier correlations is given. The paper also includes an improved correlation for the temperature dependence of the zero-density viscosity of tetrafluoromethane. of the zero-density viscosity of tetrafluoromethane.

100,362
PB91-192518
Rot available NTIS
Ecole Polytechnique, Montreal (Quebec).
Coupled Phase Diagram-Thermodynamic Analysis
of the 24 Binary Systems, A2CO3-AX and A2SO4AX Where A = Li, Na, K and X = CI, F, NO3, OH.

Bimonthly rept. Y. Dessureault, J. Sangster, and A. D. Pelton. c1990,

Sponsored by American Ceramic Society, Columbus, OH., and National Inst. of Standards and Technology,

OH., and National first of Standards and Technology, Gaithersburg, MD. Included in Jnl. of Physical and Chemical Reference Data, v19 n5 p1149-1178 Sep/Oct 90. Available from American Chemical Society, 1155 16th St., NW, Wash ington, DC. 20036-9976.

Keywords: \*Molten salts, \*Phase diagrams, Thermodynamic properties, Lithium halides, Sodium halides, Potassium halides, Chlorides, Carbonates, Fluorides, Nitrates, Sulfates, Hydroxides.

A complete bibliographic search for all thermodynamic and phase diagram data on the 24 binary systems A2CO3-AX and A2SO4-AX (where A=Li, Na, K and X=F, Cl, OH, NO3) was carried out. A computer-assisted simultaneous evaluation of all data was per-formed in order to obtain optimized equations for the thermodynamic properties of the phases. A re-evaluation of the thermodynamic data for several of the pure salts was also carried out. The optimized thermody-namic parameters are reported as well as the phase diagrams calculated from these equations. These are considered to be the best evaluated phase diagrams which can be deduced from the data currently available. Estimated error limits of all binary assessments are given.

100,363
PB91-192526
Rown Univ., Providence, RI. Div. of Engineering. Equilibrium and Transport Properties of Gas Mix-tures at Low Density: Eleven Polyatomic Gases and Five Noble Gases.

J. Bzowski, J. Kestin, E. A. Mason, and F. J. Uribe. c1990, 44p Grant NANB7-D0703

Sponsored by National Inst. of Standards and Technology, Gaithersburg, MD. Included in Jnl. of Physical and Chemical Reference Data, v19 n5 p1179-1232 Sep/Oct 90. Available from American Chemical Society, 1155 16th St., NW, Washington DC 20036 9036 ington, DC. 20036-9976.

Keywords: \*Polyatomic gases, \*Rare gases, Transport properties, Chemical equilibrium, Mixtures, Algorithms.

The paper uses results from statistical-mechanical theory, applied through a combination of an extended principle of corresponding states with some knowledge of intermolecular potentials, to the calculation of the transport and equilibrium properties of gas mix-tures at low density. The gases involved are: N2, O2, NO, CO, CO2, N2O, CH4, CF4, SF6, C2H4, C2H6, and He, Ar, Ne, Kr, Xe. The properties included are: second virial coefficient, viscosity, diffusion, and thermal diffusion, but not thermal conductivity. The calculations are internally, thermodynamically consistent and the resulting algorithms, which are fully programmable, operate in an entirely predictive mode by means of validated combination rules. The paper is a sequel to one on the five noble gases and all their possible mixtures and a second on the above eleven polyatomic gases. The paper contains ten tables (mainly intended for the checking of computer codes) and 201 graphs of deviation and comparison plots.

100,364 PB91-192534 Not available NTIS British Columbia Univ., Vancouver. Dept. of Mechanical Engineering.
Unified Fundamental Equation for the Thermody-

namic Properties of H2O.

namic Properties of H2O.

Bimonthly rept.
P. G. Hill. c1990, 42p

Sponsored by National Inst. of Standards and Technology, Gaithersburg, MD.
Included in Jnl. of Physical and Chemical Reference
Data, v19 n5 p1233-1274 Sep/Oct 90. Available from American Chemical Society, 1155 16th St., NW, Washington DC. 20036 9036 ington, DC. 20036-9976.

Keywords: \*Water, \*Thermodynamic properties, Equations of state, Compressive properties, Acoustic velocity, Specific heat, Graphs(Charts). A new unified equation of state for H2O is presented, which includes the revised and extended scaling equation of Levelt Sengers, Kamgar-Parsi, Balfour and Sengers, is continuous over all single phase states of H2O from triple point pressure and temperature to 1000 MPa (or the melting line) and 1000 C and provides accurate representation of existing thermody-namic data in that range. In addition it provides a smooth transition from singular critical region functions to the nonsingular far-field functions. This is demonstrated by the variations of isochoric specific heat, iso-thermal compressibility, speed of sound, specific heat ratio and coexistence line properties in the critical

100,365 PB91-192542 Not available NTIS

PB91-192542 Not available NTIS American Chemical Society, Washington, DC. Journal of Physical and Chemical Reference Data, Volume 19, Number 6, November-December 1990. Bimonthly rept.
D. R. Lide. c1990, 389p
See also PB91-192559 through PB91-192583. Errata sheet inserted. Prepared in cooperation with American Inst. of Physics, New York. Sponsored by National Inst. of Standards and Technology, Gaithersburg, MD. Available from American Chemical Society, 1155 16th St., NW, Washington, DC. 20036-9976.

Keywords: \*Research, Thermal conductivity, Viscosity, Rare gases, Line spectra, Stark effect, Polyatomic molecules, Molecular energy levels, Vibrational states, Organic nitrogen compounds, Amines, Thermodynamic properties, Thermophysical properties, Transient molecules.

Contents:

The Viscosity and Thermal Conductivity of Pure Monatomic Gases from Their Normal Boiling Point up to 5000 K in the Limit of Zero Density and at 0.101325 MPa;

Experimental Stark Widths and Shifts for Spectral Lines of Neutral and Ionized Atoms (A Critical Review of Selected Data for the Period 1983 through 1988);

Vibrational and Electronic Energy Levels of Polyatomic Transient Molecules Supplement 1; Thermodynamic and Thermophysical Properties of Organic Nitrogen Compounds. Part 1. Methanamine, Ethanamine, 1- and 2-Propanamine, Benzenamine, 2-, 3-, and 4-Methylbenzenamine.

100.366 PB91-192559 Not available NTIS Rostock Univ. (German D.R.), Fachbereich Chemie.

Viscosity and Thermal Conductivity of Pure Monatomic Gases from Their Normal Boiling Point Up to 5000 K in the Limit of Zero Density and at 0.101325 MPa.

Birmonthly rept.
E. Bich, J. Millat, and E. Vogel. c1990, 17p
Sponsored by National Inst. of Standards and Tech-

nology, Gaithersburg, MD. Included in Jnl. of Physical and Chemical Reference Data, v19 n6 p1289-1306 Nov/Dec 90. Available from American Chemical Society, 1155 16th St., NW, Washington, DC. 20036-9976.

Keywords: "Thermal conductivity, "Viscosity, "Helium, \*Neon, \*Argon, "Krypton, "Xenon, Transport proper-ties, Kinetic theory, Tables(Data).

The kinetic theory of gases in the limit of zero density and that of moderately dense gases is used to generate accurate tables of the viscosity and thermal conductivity of the pure monatomic gases for zero density and for a pressure of 0.101325 MPa. The theoretically-based tables cover the temperature range from the normal boiling point of the relevant gas up to 5000 K. The associated uncertainties of the proposed data are detailed in the paper. A comparison of the correlated data with experimental results and some other recent correlations is given.

PB91-192575 Not available NTIS
National Inst. of Standards and Technology (NML),
Gaithersburg, MD. Molecular Physics Div. Vibrational and Electronic Energy Levels of Polyatomic Transient Molecules. Supplement 1.

Bimonthly rept. M. E. Jacox. c1990, 160p

Sponsored by National Inst. of Standards and Technology, Gaithersburg, MD.

Included in Jnl. of Physical and Chemical Reference Data, v19 n6 p1387-1546 Nov/Dec 90. Available from American Chemical Society, 1155 16th St., NW, Washington, DC. 20036-9976.

Keywords: \*Polyatomic molecules, \*Molecular energy levels, \*Vibrational states, Laser induced fluoreslevels, \*Vibrational states, Laser induced fluores-cence, Photoelectron spectroscopy, Emission spectra, Free radicals, Infrared spectra, Hydrides, Matrix isolation, Molecular ions, Radiative lifetime, Raman spectra, Ultraviolet absorption, Tables(Data), \*Transient molecules.

New information on the experimentally determined vibrational and electronic energy levels of approximately 500 neutral and ionic transient molecules possessing from 3 to 16 atoms has been evaluated and added to the previously established database for these species. There has been selective extension of the compilation to somewhat less reactive species such as HNCO, HCNO, H2O2, and cis- and trans-HONO, as well as to many transient molecules which include atoms beyond the third row of the Periodic Table. Electronic spectral data are also given for a number of transient mole-cules which possess more than six atoms. Radiative life-times and the principal rotational constants are included. Observations in the gas phase, in molecular beams, and in rare-gas and nitrogen matrices are eval-uated. The types of measurement surveyed include conventional and laser-based absorption and emission techniques, laser absorption with mass analysis, and photoelectron spectroscopy.

100.368 PB91-192583 Not available NTIS Texas A and M Univ., College Station. Thermodynamics Research Center.

Thermodynamic and Thermophysical Properties of Organic Nitrogen Compounds. Part 1. Methanamine, Ethanamine, 1- and 2-Propanamine, Benzenamine, 2-, 3-, and 4-Methylbenzenamine.

Bimonthly rept.

J. Chao, N. A. M. Gadalla, B. E. Gammon, K. N.
Marsh, A. S. Rodgers, G. R. Somayajulu, and R. C.
Wilhoit. c1990, 70p

Sponsored by National Inst. of Standards and Tech-

nology, Gaithersburg, MD.
Included in Jnl. of Physical and Chemical Reference
Data, v19 n6 p1547-1616 Nov/Dec 90. Available from
American Chemical Society, 1155 16th St., NW, Washington, DC. 20036-9976.

Keywords: \*Organic nitrogen compounds, \*Amines, \*Thermodynamic properties, \*Thermophysical properties, Boiling points, Freezing, Critical point, Specific heat, Vapor pressure, Enthalpy, Vaporization, Virial coefficients, Density, Combustion, Thermochemistry.

The thermodynamic and thermophysical properties of eight primary amines, methanamine, ethanamine, 1-and 2-propanamine, benzenamine, and 2-, 3-, and 4-methylbenzenamine have been evaluated. Recommended values are given for the following properties: normal boiling, freezing, and triple-point temperatures, critical constants, thermodynamic properties in the solid and liquid phases, vapor pressure, enthalpy of vaporization, density, second virial coefficients, and enthalpy of combustion. Ideal gas thermodynamic properties have been calculated by statistical mechanical methods.

100,369

PB91-194472 PC A04/MF A01 National Inst. of Standards and Technology (CSTL), Gaithersburg, MD.

Experimental Thermal Conductivity, Thermal Diffusivity, and Specific Heat Values for Mixtures of Nitrogen, Oxygen, and Argon.

Final rept.
R. A. Perkins, and M. T. Cieszkiewicz. Mar 91, 65p. NISTIR-3961

See also PB89-148407. Sponsored by Wright Research and Development Center, Wright-Patterson AFB, OH., and National Aeronautics and Space Administration, Cleveland, OH. Lewis Research Center.

Keywords: \*Thermal conductivity, \*Thermal diffusivity, \*Specific heat, \*Ternary systems, \*Nitrogen, \*Oxygen, \*Argon, Binary system(Materials), Hot wire anemometers, Tables(Data), Temperature dependence, Pressure dependence, Standards, Thermodynamic properties, Measurement, Supercritical state, Mixture Equations of active Correlations (Liquidical tures, Equations of state, Correlations, Liquefied gases, Air.

# Physical & Theoretical Chemistry

Experimental measurements of thermal conductivity and thermal diffusivity obtained with a transient hotwire apparatus are reported for three mixtures of nitrogen, oxygen, and argon. Values of the specific heat, Cp. are calculated from these measured values and the density calculated with an equation of state. The measurements were made at temperatures between 65 and 303 K with pressures between 0.1 and 70 MPa. The data cover the vapor, liquid, and supercritical gas phases for the three mixtures. The total reported points are 1066 for the air mixture (78.11% nitrogen - 20.97% oxygen - 0.92% argon), 1058 for the 50% nitrogen - 50% oxygen mixture, and 864 for the 25% nitrogen - 75% oxygen mixture. Empirical thermal conductivity correlations are provided for the three mix-

100.370 PB91-194837 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Molecular Spectroscopy Div. Theoretical Model of Metal Binding Sites in Proteins. Final rept.

M. Krauss, and W. J. Stevens. 1989, 13p Pub. in Progress in Clinical and Biological Research 289, p95-107 1989.

Keywords: \*Subtilisins, \*Molecular orbitals, \*Binding energy, \*Calcium ions, \*Magnesium ions, \*Sodium ions, Proteins, Cations, Metals, Reprints, \*Binding

Ab initio molecular orbital calculations of the binding energy of metal cations to clusters of water, formamenergy of metal cations to clusters of water, formamide, and formate ligands are used to analyze Ca binding sites in proteins. The ab initio energetics of the first coordination shell provide a basis for evaluating the conformation behavior and the selectivity of cation binding. The enthalpies of binding are modeled by estimating the Born polarization energy relative to the model cluster of the first shell. The data is applied to an analysis of binding sites in the protein, Subtilisin BPN. In the study the Ca, Mg, and Na cation energetic selectivity is compared for binding to two of the sites.

100,371 PB91-194944 Not available NTIS National Inst. of Standards and Technology (IMSE),

Gaithersburg, MD. Ceramics Div.
Reflection-Extended-X-ray-Absorption-FineStructure Spectroscopy at the Carbon K-Edge. Final rept.

G. G. Long, D. R. Black, and D. K. Tanaka. 1989, 6p Pub. in Materials Research Society Symposia Proceedings, v143 p157-162 1989.

Keywords: \*Glassy carbon, Graphite, Chemical bonds, Vitreous state, Backscattering, Reprints, Extended X-ray absorption fine structure spectroscopy, K-edge

The carbon K-edge Reflection-Extended X-Ray Absorption Fine Structure (refl-EXAFS) spectra from graphite, diamond and glassy carbon have been investigated. There is good phase shift transferability between the two well-known bonding types in diamond and graphite, provided that appropriate inner potential corrections to the K-edge (E(sub o) are made. The model spectra from diamond and graphite were used to investigate the nature of glassy carbon. It was found that, for the particular form of glassy carbon used in the study, the bonding more closely resembled sp3 than sap2. The result is preliminary pending the authors' evaluation of the influence of surface oxygen.

100.372 Not available NTIS PB91-194951 National Inst. of Standards and Technology (IMSE), Gaithersburg, MD. Ceramics Div.

Surface-Extended X-ray-Absorption Fine-Struc-ture Experiments at Atmospheric Pressure by Means of a Photocathode Proportional Counter with Monolayer Sensitivity.

G. G. Long, D. K. Tanaka, J. Kruger, G. A. Danko, and D. A. Fischer. 1989, 7p Pub. in Physical Review B 39, n15 p651-657 1989.

Keywords: \*Iron oxides, X-ray absorption, Proportional counters, Photocathodes, Thin films, Substrates, Surfaces, Reprints.

Surface-EXAFS (extended x-ray absorption fine structure) measurements at atmospheric pressure were made by means of a new photocathode proportional counter on the oxide films that form on bulk iron substrates. Both thermally-formed and chemically-formed films were studied. Near-edge spectra with effective monolayer sensitivity were used to investigate the ionicity of cations in ultra-thin films.

100.373 PB91-194985 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Center for Chemical Technology. PLOTMD: An Interactive Program to Modify Molecular Plots on a Graphics Terminal. Final rept.

J. C. Luo, G. L. Gilliland, and H. L. Ammon. 1989, 1p Pub. in Jnl. of Applied Crystallography 22, p186 Apr 89.

Keywords: \*\*Crystallography, \*Stereochemistry, \*Graphic methods, \*Crystal structure, \*Computer programs, Molecular structure, Reprints, PLOTMD pro-

A program was written to display an HP 7550A plot file on a MicroVax II workstation. Some of the modifications of the picture that can be performed are: (1) change between 8.5 x 11 and 11 x 8.5 inch formats; (2) rotate about Z-axis; (3) move picture up-down and rotate about 2-axis; (3) move picture up-down and right-left; (4) increase or decrease picture size; (5) insert dashed lines between atoms, perhaps to indicate a weak interaction; (6) manipulate labels. Labeltext information can be deleted, inserted, moved, altext information can be deleted, inserted, moved, altered and increased or decreased in size. Stereo-labeling is carried out automatically from manipulations on the left-eye image. The program is written in VAX FORTRAN(V4.0) on the MicroVMS operating system(V4.5). The graphics procedures are based on the MicroVMS workstation graphics software(V3.0). The program is implemented on a standard MicroVAX II workstation with a 20 inch monochrome monitor and a mouse. a mouse.

PB91-195008 Not available NTIS National Inst. of Standards and Technology (IMSE), Gaithersburg, MD. Metallurgy Div. Atomistic Diffusion Equations and Kinetic Forces.

J. R. Manning. 1989, 15p Sponsored by Office of Naval Research, Arlington, VA. Pub. in Diffusion Analysis and Applications, p3-17

Keywords: \*Diffusion, \*Reaction kinetics, Thermodynamic equilibrium, Metals, Theories, Equations, Vacancies, Crystal structure, Reprints.

There are two major approaches to diffusion theory, (1) the atomistic-kinetic approach in which the motions of individual atoms are followed and (2) the continuum-thermodynamic approach in which thermodynamic forces are described which move the system toward an equilibrium state by inducing atom fluxes. In the present paper, atomistic-kinetic diffusion equations are developed from a consistent point of view based on calculations of the energy change resulting from in-dividual atom jumps. The approach, which is generally applicable, is employed here to give for the first time a fully atomistic calculation of kinetic driving forces from coherency strains, the energy of mixing and the gradi-ent energy. Effects on the kinetic equations from vacancy concentration gradients, vacancy fluxes and dependencies of vacancy formation energy on composi-tion are also calculated; and a general atomistic-kinet-ic expression for the atom flux between neighboring planes is developed. The equation is shown to provide the same type of forces and terms as those in the gen-eral thermodynamic diffusion equations. Thus, the two approaches yield identical results. They can be usefully combined to provide practical applications of diffusion theory that would not be obtained from either approach alone.

100,375 PB91-195065 Not available NTIS National Bureau of Standards (NML), Gaithersburg,

MD. Chemical Kinetics Div.
Carbon Acidities of Aromatic Compounds. 2. Ionic Probes of Aromaticity in Annelated Rings.

M. Mautner, J. F. Liebman, and S. A. Kafafi. 1988, 5p Pub. in Jnl. of the American Chemical Society 110, n18

p5937-5941 1988.

Keywords: \*Aromatic compounds, \*Chemical bonds, \*Aromatic polycyclic hydrocarbons, \*Hydrogen ions 1

plus, Acidity, Carbon, Atomic models, Resonance charge exchange, Benzene, Pyridines, Ionization, Polarizability, Napthalene, Indene, Semiempirical equations, Stability, Reprints, Protonation, Annelation, Charge stabilization.

lonization by the deprotonation of benzene and pyridine, and by the protonation of pyridine, involve lone pairs in the sigma plane without significant pi effects. In pairs in the sigma plane without significant pletrects. In these case annelation by a benzene ring increases the acidity or proton affinity by a constant 6 + or - 1 kcal/mol, ascribed to increased polarizability. In com-parison, protonation of benzene and deprotonation of cyclopentadiene disrupts or creates a 6-electron aromatic system, respectively, and in their annelated de-rivatives, naphthalene and indene, a secondary 4-elec-tron conjugated pi system. These cases involving pi electrons show annelation effects that are substantially larger (13.4 kcal/mol) or smaller (1.0 kcal/mol) respectively, than just the electrostatic effect. Analysis of these data suggests that the stability of secondary 4electron systems in the annelated rings is smaller by 6 + or - kcal/mol than the aromatic 6-electron systems. In fair agreement with Herndon's structure resonance values for these species. Annelation effects are reproduced well by Dewar's AM1 semiempirical method.

100.376 Not available NTIS
National Inst. of Standards and Technology (NML),
Gaithersburg, MD. Chemical Kinetics Div.
Thermal Decomposition of lone 3. Proceedings of the composition of lone 2. Thermal Decomposition of Ions. 3. Protonated Ethanol and Diethyl Ether.

M. Mautner, and L. W. Sieck. 1989, 11p See also PB87-162301. Pub. in International Jnl. of Mass Spectrometry and Ion Processes 92, p123-133 1989.

Keywords: \*Organic ions, \*Ethanol, \*Ethyl ether, \*Pyrolysis, Reaction kinetics, Activation energy, Protons, Reprints.

Above 550 K, the C2H5OH2+ ion decomposes to yield H3O+ with the loss of C2H4. An alternative decomposition channel is the formation of CH3CHOHwhere in the H2 lost, deuteration studies suggest that where in the H2 lost, deuteration studies suggest that one hydrogen atom originates from hydroxyl and another from the ethyl group. The decomposition products regenerate C2H50H2+ by proton transfer to C2H50H, forming reaction cycles that reach steady-states. At higher concentrations of C2H50H, condensation with C2H50H2+ forms (C2H5)2OH+, which in C2H50H2+, resulting in another steady-state cycle. Decomposition rate constants are calculated from steady-state ion ratios, and 150-670K are in the range of 1 to 100000/sec for all the reactions. The decompoof 1 to 100000/sec for all the reactions. The decompositions of C2H5OH2+ are at the low-pressure limit and of (C2H5)2OH+ are at the high-pressure limit at 2 - 8 torr. The decompositions show Arrhenius activation energies of 10 to 30K cal/mol.

100.377 PB91-195131 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Thermophysics Div. Dipole Moments of Seven Partially Halogenated

Ethane Refrigerants.

Final rept. C. W. Meyer, and G. Morrison. 1991, 7p Pub. in Jnl. of Physical Chemistry 95, n9 p3860-3866, 2 May 91.

Keywords: \*Refrigerants, \*Fluorinated alphatic hydrocarbons, \*Ethane, \*Dipole moments, \*Gases, Temperature dependence, Refractivity, Measurement, Dielectric properties, Polarizability, Reprints.

Dielectric constant measurements have been performed on seven partially halogenated ethanes, currently being considered as alternative refrigerants, in the gaseous state over the range 305-415 K in order to determine their dipole moments. Argon was also studied to test the apparatus. Five of the refrigerants have temperature-independent moments: R125 (CF3CHF2), mu = 1.563 + or - 0.005 D; R134a (CF3CH2F), mu = 2.262 + or - 0.008 D; and R124 (CF3CHCIF), mu = 1.469 + or - 0.012 D. Two refrigerants have conformer-dependent moments, making their time-averaged moments temperature dependent: R134 (CHF2CHF2), with a moment ranging from 0.991 + or - 0.004 D at 309 K to 1.250 + or - 0.004 D at 31 K; and R143 (CHF2CH2F), where the moment ranges

from 1.680  $\pm$  or - 0.001 D at 309 K to 1.745  $\pm$  or - 0.001 D at 410 K. Accurate estimation of a molecule's temperature-dependent dipole moment requires an independent determination of its polarizability; this determination has been made from index of refraction measurements. Where possible, the present results are compared with earlier determinations of dipole moments. In all but one instance, the agreement is good.

100,378 PB91-195214 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Chemical Kinetics Div. Proton Affinities and pKa Values of Tetraalkylhy-

drazines

Final rept S. F. Nelsen, M. Mautner, D. T. Rumack, and L. W.

Sieck. 1988, 6p Pub. in Jnl. of the American Chemical Society 110, n19 p6303-6308 1988.

Keywords: \*Hydrazine, \*Proton affinity, \*Pyridines, \*Dissociation, \*Tertiary amines, Alkyl compounds, Amines, Thermodynamic quilibrium, Solvation, Hydrogen ions 1 plus, Reprints, Proton affinity, Protonation.

Proton affinities for 16 saturated tetraalkylhydrazines were determined by equilibration with triethylamine, 2,6-dimethyl pyridine, and 2,6-diethylpyridine using high pressure mass spectrometry, and pKa measure-ments in water were made for the 14 compounds which proved soluble enough. Proton transfer equilibria for these compounds are compared with electron transfer equilibria previously measured.

100.379 PB91-195230 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Chemical Kinetics Div. Rate Constants for Reduction of Substituted Meth-

ylperoxyl Radicals by Ascorbate lons and N,N,N',N'-Tetramethyl-Para-Phenylenediamine. Final rept.

P. Neta, S. Steenken, L. V. Shastri, R. E. Huie, S. Mosseri, J. P. Mittal, and P. Maruthamuthu. 1989, 6p Pub. in Jnl. of Physical Chemistry 93, n10 p4099-4104

Keywords: \*Reaction kinetics, \*Reduction(Chemistry), \*Free radicals, Ascorbic acid, lons, Peroxy radicals, Radiolysis, Thermodynamic equilibrium, Pulse techniques, Alkyl compounds, Reprints, Tetramethyl-phenylenediamine, Taft constants.

Absolute rate constants (k) for reduction of substituted methylperoxyl radicals by ascorbate ions and by TMPD (N,N,N',N'-tetramethyl-p-phenylenediamine) in aqueous solutions have been determined by pulse radiolysis. The rate constants vary from 10 to the 6th power to 10 to the 9th power/M/s, increasing as the electron withdrawing capacity of the substituent on the peroxyl group increases. Linear correlations are observed between log k and the Taft substituent constants sigma\* for a wide variety of substituents, but not all substi-tuents fit the same line. In the case of ascorbate as reductant, the points for peroxyl radicals that contain halogens on the alpha-carbon lie on a different line (rho $\overset{*}{=} 0.41$ ) than that for the other substituents (rho $\overset{*}{=} 1.25$ ). In the case of TMPD there are also two families of peroxyl radicals: those comprising the electron donating groups Me through t-Bu (rho\* = 5.6) and those containing electron-withdrawing substituents (rho\* = 0.64).

PB91-195255 Not available NTIS National Bureau of Standards (IMSE), Gaithersburg, MD. Reactor Radiation Div. Dynamics of Molecular Hydrogen Adsorbed in

CoNa-A Zeolite. Final rept.

J. M. Nicol, J. Howard, and J. Eckert. 1988, 5p Pub. in Jnl. of Physical Chemistry 92, n25 p7117-7121 1988

Keywords: \*Hydrogen, \*Adsorption, \*Zeolites, Cobalt ions, Sodium ions, Neutron scattering, Chemical bonds, Reprints, \*Molecular dynamics, Vibrational spectra.

The dynamics of molecular hydrogen adsorbed in the cavities of partially cobalt exchanged type A zeolite (Co4.1Na3.8-A) has been investigated in the energy range 0-40 meV by incoherent inelastic neutron scattering. Both rotational and vibrational excitations are identified in the spectra. The rotational tunnel splitting

of the vibrational ground state of the coordinated molecular hydrogen is observed at 3.8 meV. Analysis of the data in terms of a twofold cosine potential with two degrees of rotational freedom suggests that the hydrogen molecules are bound end-on to the Co cations and perform 180 deg. reorientations with a barrier of 55-68 meV (1.3-1.5 Kcal/mole). A mode at 15.3 meV is identified as a vibration of the bound hydrogen. Evidence for the torsional mode of AI(OH)4 complexes, formed in the beta-cages during ion-exchange, is found in the vibrational spectra at 21 meV.

100 381 PB91-195297 Not available NTIS National Bureau of Standards (NML), Gaithersburg,

MD. Quantum Metrology Group.

Anomalous Th M3O1 X-ray Emission Spectrum of ThO2.

M. Ohno, and R. E. LaVilla. 1988, 4p Pub. in Physical Review B 37, n18 p915-918 1988.

Keywords: \*Thorium oxides, \*X ray spectra, Emission spectra, Greens function, Coster-Kronig transitions, Reprints.

The Th M3O1 (triplet P(3/2)(sup -1) -> 5s(sup -1)) x-ray emission spectrum (XES) of ThO2 was measured with a high resolution vacuum double crystal spectrometer. The spectrum is the first evidence of the splitting of a 5s hole level into two main structures which are due to a strong configuration interaction; 5s(sup -1) <--> 5p(sup -1)5d(sup -1)5(n, epsilon) f super Coster-Kronig process. The O(1a) and O(1b) hole energies of ThO2 determined by the present measurements are respectively, 293.9 and 276.2 eV. A large energy shift (order of about 15 eV) to lower binding energy from the theoretically predicted atomic energies is observed even when one takes into account the atom-oxide energy shift. The cause of discrepancy is suggested to be due to a strong configuration interaction of the final 5p5d double hole.

100.382 PB91-195305 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Quantum Metrology Div.

Many Electron Effects in Lgamma2,3 X-ray Emission Spectroscopy Spectrum of BaO.

Final rept. M. Ohno, and R. E. LaVilla. 1989, 7p

Pub. in Physical Review B 39, n13 p8845-8851 1989.

Keywords: \*Barium oxides, \*X ray spectra, Coster-Kronig transition, Emission spectra, Greens function, Reprints.

The L(gamma 2,3)(2s(sup -1) -> 4p(sup -1) x-ray emission spectrum (XES) of BaO was measured in fluorescence with a high resolution vacuum double crystal spectrometer. The spectrum was also calculated by the Green's function method. It is shown that the spectrum can be interpreted essentially in terms of a two level system in the final state, e.g., the 4p hole level interacting with the product of the 4p(sup -1) <--> 4d(sup -2)4f super Coster-Kronig process. It is also shown that it is necessary to take into account the 4d(sup -2)4f multiplet.

100.383 PB91-195313 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Quantum Metrology Div.

Many-Electron Effects in Lgamma2,3 XES Spectra from Rare Earth Elements. Final rept.

M. Ohno, and R. E. LaVilla. 1989, 6p Pub. in Physical Review B 39, n13 p8852-8857 1989.

Keywords: \*Neodymium oxides, \*Samarium oxides, \*X ray spectra, Coster-Kronig transitions, Emission spectra, Greens function, Reprints.

The L(gamma 2,3)(2s(sup -1)->4p(sup -1)) x-ray emission spectra of Nd2O3 and Sm2O3 were measured in order to study the strong configuration interaction between a 4p hole level and the double 4d hole  $4f(\sup n+1)$  electron levels. The spectra are calculated also using the Green's function method. The agreement between theory and experiment is reasonably good. The spectrum can be interpreted in terms of the spectral function of the final 4p hole where it is shown that the one-electron picture of the 4p hole breaks down due to the strong  $4p(\sup -1) <-> 4d(\sup -2) 4f(\sup n+1)$  super Coster-Kronig process.

100.384 PB91-195370 Not available NTIS National Inst. of Standards and Technology (NML),

Gaithersburg, MD. Chemical Kinetics Div.

Reactions of C5H3(+) and C5H5(+) lons with
Acetylene and Diacetylene.

Final rept. F. Ozturk, S. G. Lias, M. Moini, F. W. Brill, and T. J. Buckley. 1989, 7p See also AD-A197 087.

Pub. in Jnl. of Physical Chemistry 93, n10 p4038-4044

Keywords: \*Acetylene, \*Alkene compounds, \*Alkyne compounds, Ion cyclotron-resonance, Reaction kinetics, Reprints, \*Organic ions, \*Diacetylene, \*Butyne, Fourier transform mass spectroscopy, Ion molecule re-

The reactions of C5H3(1+) and C5H5(1+) ions with acetylene and diacetylene were investigated using a Fourier transform ion cyclotron resonance (FTICR) mass spectrometer. The ejection capabilities of FTICR were used to determine the reaction mechanisms and rate constants for the reactions of ions produced from a number of different precursors. While different structures could be attributed to C5H3(1+) ions produced from different precursors on the basis of reactivity, no significant differences in the rate constants of C5H5(1+) ions were observed. Different percentages of reactive C5H5(1+) structure(s) were produced from different precursors using different charge transfer gases. Formation of C5H5(1+) from norbornadiene and cycloheptatriene was studied in more detail and existence of a second formation mechanism was shown to be possible.

100.385

PB91-195735 Not available NTIS National Bureau of Standards (IMSE), Gaithersburg, MD. Ceramics Div.

High-Temperature High-Pressure Raman Spectra from Liquid Water.

Final rept.

G. E. Walrafen, W. H. Yang, M. S. Hokmabadi, and G. J. Piermarini. 1988, 3p Pub. in Jnl. of Physical Chemistry 92, n15 p4540-4542

Keywords: \*Raman spectra, \*Water, Hydrogen bonds, Pressure dependence, High pressure, High temperature, Reprints, Diamond anvils.

Raman spectra were obtained from liquid water at 33 kbar and at 170 and 200 C using a diamond anvil cell. Pressures were determined from the ice VII-water melting temperatures. Comparison of the present data, with data from Lindner and Franck, indicates that the OH-stretching peak frequency, in cm(sup -1), decreases with increasing pressure at constant temperature. Further analysis of the data suggests that the double-to-single, hydrogen-bond potential-well trans-formation, which is known to occur for linear hydrogen bonds, also occurs for severely bent, nonhydrogenbonded, O-H-O configurations.

100,386 PB91-200782 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Chemical Kinetics Div. Reactivities of Chlorine Atoms and Peroxyl Radi-

cals Formed in the Radiolysis of Dichloromethane. Final rept Z. B. Alfassi, S. Mosseri, and P. Neta. 1989, 6p

Sponsored by Department of Energy, Washington, DC. Pub. in Physical Chemistry 93, n4 p1380-1385 1989.

Keywords: \*Methylene chloride, \*Peroxy radicals, \*Chlorine, \*Atoms, \*Reactivity, \*Reaction kinetics, Radiolysis, Anilines, Chemical radicals, Phenols, Hydrogen transfer, Ethers, Reprints.

Radiolysis of dichloromethane (DCM) leads to formation of primary oxidizing radicals and carbon-centered radicals. The latter react with oxygen to yield peroxyl radicals. The yields and chemical behavior of these intermediates were studied by pulse radiolysis of DCM solutions containing various solutes: phenols, anilines, dimethoxybenzene, hexamethylbenzene, cyclohexene, dimethyl sulfoxide, and zinc tetratolylporphyrin. At low concentrations, some of these solutes were found to be oxidized by two peroxyl radicals, CHClO2(dot) and CHCl2O2(dot), with different rate constants. At higher concentrations, the solutes react also with the

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primary radicals: CI atoms and the radical cations CH2CI2(+, dot) with diffusion-controlled rate constants. The rates of these reactions were determined by competition kinetics because of the very short life-times of the species. CI atoms were found to have a half-life of about 5 ns in DCM, reacting predominantly with the solvent by hydrogen abstraction. The radical cations decay within a fraction of a nanosecond. The total yield of these primary radicals was determined to be G=3.6 and appears to be divided about equally between CI and the radical cations. The total yield of oxidation, by the primary and the peroxyl radicals, was found to be G=7.5. Cl atoms were found to be very reactive in electron transfer as well as addition and hydrogen abstraction reactions.

Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Molecular Spectroscopy Div. 100,387 PB91-202846

Time- and State-Resolved Measurements of Nitric Oxide Dimer Infrared Photodissociation.

Final rept. M. P. Casassa, J. C. Stephenson, and D. S. King. 1988, 11p Pub. in Jnl. of Chemical Physics 89, n4 p1966-1976

Keywords: \*Nitric oxide, \*Photodissociation, Laser induced fluorescence, Van der Waals forces, Vibrational states, Picosecond pulses, Infrared spectra, Predissociation, Lifetime, Dimers, Reprints.

Picosecond and nanosecond lasers and pulsed molecular beam techniques have been used to measure the infrared photodissociation spectra, the product state distributions, and the predissociation lifetimes of vibrationally excited nitric oxide dimer, (NO)2. Results for the nu(1)(v=1) symmetric NO stretching mode and the nu(4)(v=1) antisymmetric NO stretching mode are presented. Predissociation lifetimes are determined by time-resolved laser induced fluorescence probing of the NO monomer product appearance rate. The observations are discussed in terms of various vibrational predissociation mechanisms, including vibrational potential coupling and electronically nonadiabatic predissociation.

100,388 PB91-202853 Not available NTIS National Bureau of Standards (IMSE), Gaithersburg, MD.

Grain Boundaries in a 2-D Superlattice. Final rept.

P. Cenedese, R. Kikuchi, and J. W. Cahn. 1988, 6p Pub. in Materials Research Society Symposium Proceedings 122, p231-236 1988.

Keywords: \*Crystal structure, \*Grain boundaries, \*Superlattices, \*Bicrystals, Cluster analysis, Predictions, Two-dimensional calculations, Microstructure, Thermodynamic properties, Mathematical models, Gases, Dihedral angle, Wetting, Transition temperature, Critical tomacrature, Transcription temperature, Critical tomacrature, Transcription and Company (1997). cal temperature, Temperature dependence, Adsorption, Reprints.

In bicrystals with CSL orientation relationships two kinds of coincidence site lattices form, resulting in two kinds of grain boundaries. The thermodynamic properties are examined, using a lattice gas model, and make microstructural predictions about the dihedral angles at junctions between these boundaries. The behavior of these boundaries is examined for low temperatures and through the critical disordering temperature. Some aspects of nonstoichiometry are presented. A wetting transition is found at low temperatures, in which one kind of grain boundary is converted into the other by expelling antiphase domain boundary. No wetting transition is found at the critical temperature because an unusually high critical exponent of 3 is found for the difference in grain boundary energies between the symmetric and antisymmetric cases.

100,389 PB91-202986 Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Quantum Physics Div. Causes of SiH4 Dissociation in Silane dc Discharges.

Final rept. D. A. Doughty, and A. Gallagher. 1990, 5p Contract SERI-XB-2-02189

Sponsored by Solar Energy Research Inst., Golden,

Pub. in Physical Review A 42, n10 p6166-6170, 15 Nov

Keywords: \*Silane, \*Gas discharges, \*Chemical dissociation, lon-molecule collisions, Silicon hydrides, Amorphous silicon, Semiconducting films, Substrates, Glass, Reprints.

Hydrogenated amorphous-silicon (alpha-Si:H) film growth on glass fibers strung between discharge electrodes is used to measure the distribution of film-producing radicals in a silane dc discharge. The measured distribution, as well as film deposition rates on the electrodes, show that typically > 80% of the depositing radicals are produced in the cathode sheath. Discharge models, confirmed by the spatial distribution of control emission rule out the possibility that this discontrol. optical emission, rule out the possibility that this disso-ciation in the sheath is due to electron impact. Collisions of energetic ions and neutrals with silane are clearly implicated as the cause of the sheath dissocia-tion. In contrast, due to much lower ion kinetic energies, almost all dissociation is due to electron collisions in the low-power rf discharges most commonly used for film production. In addition, the ratio of the number of Si atoms deposited on all surfaces to the total number of ions collected at the dc-discharge cathode is measured to be 30, demonstrating the dominance of neutral radical deposition in these discharges.

100,390 PB91-202994 Not available NTIS Notional Inst. of Standards and Technology (NML), Boulder, CO. Quantum Physics Div. Silane Dissociation Products in Deposition Discharges. Final rept.

J. R. Doyle, D. A. Doughty, and A. Gallagher. 1990, 10p

Contract SERI-XG-1-1216

Sponsored by Solar Energy Research Inst., Golden,

Pub. in Jnl. of Applied Physics 68, n9 p4375-4384, 1 Nov 90.

Keywords: \*Silane, \*Gas discharges, \*Chemical dissociation, Surface reactions, Amorphous silicon, Semi-conducting films, Reprints.

Time-dependent production of higher-silane gases and alpha-Si:H film are measured relative to decomposed silane in rf and dc, hot and cold cathode, staticgas discharges. From the absence of higher-silane production in very low silane partial-pressure discharges, it is inferred that most higher silanes are produced by gas-phase SiH2-initiated reactions. The duced by gas-phase SiH2-initiated reactions. The higher silanes are thus tracers of SiH2, while the film production traces the fraction of H, SiH, and SiH3 in the initial decomposition. From the measured stable product yields, the authors deduce that SiH4 -> SiH2 + 2H is the dominant electron-collisional dissociation channel.

PB91-203018 Not available NTIS
National Bureau of Standards (NML), Gaithersburg,
MD. Chemical Kinetics Div.
Ultraviolet Absorption of the Vinyl Radical and Reaction with Oxygen.

Final rept.

A. Fahr, and A. H. Laufer. 1988, 4p Pub. in Jnl. of Physical Chemistry 92, n26 p7229-7232

Keywords: \*Vinyl radicals, \*Ultraviolet spectra, Photolysis, Reaction kinetics, Fan ultraviolet radiation, Absorptivity, Oxygen, Reprints.

Two absorption features at 1647.1A and 1683.3A have been detected from the vacuum ultraviolet flash photolysis of either Sn(C2H3)4 or Hg(C2H3)2. The features are assigned to the vinyl radical. Extinction coefficients of 1150 + or - 500/cm/atm and 1120 + or - 500/cm/atm (base e) for the two bands, respectively, have been measured and a rate constant of (6.7 + or 2.7 x 10 to the -12)cc/molec/sec for the reaction of C2H3 + 02 has been determined.

PB91-203034 Not available NTIS National Inst. of Standards and Technology (IMSE),

Caithersburg, MD. Ceramics Div.

Lanthanide Coordination Chemistry: Spectroscopic Properties of Terbium and Europium Poly(Pyrazol-1-YI) Borate and Poly(Imidazol-1-YI) Borate.

Final rept.

R. A. Faltynek. 1989, 8p Pub. in Jnl. of Coordination Chemistry 20, n1 p73-80

Keywords: \*Lanthanum complexes, \*Spectrum analysis, \*Borates, \*Terbium complexes, \*Europium complexes, Charge transfer, Infrared spectra, Ultraviolet spectra, Imidazoles, Pyrazoles, Luminescence, Ligands, Electron spectroscopy, Reprints.

Complexes formed between poly(pyrazol-1-yl) - or poly(imidazol-1-yl) borate anions and tripositive cations of terbium or europium were examined by infrared, UV absorption, and emission spectroscopy. Trisand tetrakis(heterocycle)borates yielded isostructural and tetrakis(heterocycle)borates yielded isostructural compounds with both lanthanides, having a different molecular geometry than the bis(heterocycle)borate complexes. Electronic spectra indicate that the poly(pyrazol-1-yl)borate complexes emit from a ligand-to-metal (LMCT) charge transfer state. The free ligands are UV transparent however, suggesting that the sensitizing chromophore responsible for emission is created only upon complexation. The polylimidazolis created only upon complexation. The poly(imidazol-1-yl)borate compounds, exhibit a more complex excited state profile, with emission apparently originating from both LMCT and intraligand states.

100 393

PB91-203075 Not available NTIS Not available NTIS
National Inst. of Standards and Technology (NEL),
Gaithersburg, MD. Chemical Process Metrology Div.
Chemical and Electronic Properties of Pd/
SnO2(110) Model Gas Sensors. Final rept.

T. B. Fryberger, J. W. Erickson, and S. Semancik.

1989, 7p Pub. in Surface and Interface Analysis 14, n1-2 p83-89 Jan/Feb 89.

Keywords: \*Catalysts, \*Palladium, \*Tin oxides, \*Vapor deposited coatings, \*Ceramics, \*Gas detectors, Metal films, Solid-solid interfaces, Monomolecular films, Annealing, Surface chemistry, Surface resistivity, Metalography, Hydrogen, Time dependence, Pressure dependence, Chemical properties, Electronic structure, Scattering, Reprints.

The Pd/SnO2(110) interface has been investigated as a model gas sensor system. Techniques including XPS, UPS, ISS, and 4-point conductivity measurements were used to study the growth mode and chemical interaction of Pd with this SnO2 surface for coverages between 0.1 and 10.0 monolayer-equivalents (ML-EQ). It was found that the Pd overlayer grows by clustering at 300K and that the deposited Pd is primarily metallic by 3 ML-EQ. Heating Pd-covered surfaces up to 800K causes a decrease in the XPS Pd/Sn 3d intensity ratio, possibly due to further clustering of the intensity ratio, possibly due to further clustering of the overlayer above room temperature. Annealing did not, however, change the metallic nature of the deposited Pd. The gas sensing behavior of these model surfaces was tested by measuring the surface conductivity vs. time at several hydrogen pressures and the conductivity response for a 3 ML-EQ Pd/SnQ2(110) surface was found to be 16 times greater than that for the Pd-free surface.

100,394

PB91-203232 Not available NTIS National Inst. of Standards and Technology (NML),

Raithersburg, MD. Chemical Kinetics Div.
Rate Constants for Hydrogen Abstraction Reactions of the Sulfate Radical, SO4- Alkanes and Ethers.

Final rept. R. E. Huie, and C. L. Clifton. 1989, 9p Pub. in International Jnl. of Chemical Kinetics 21, n8 p611-619 Aug 89.

Keywords: \*Sulfates, \*Radicals, \*Hydrogen trasfer, \*Reaction kinetics, \*Alkanes, \*Ethers, Photolysis, Persulfate, Chemical reactions, Reprints.

Rate constants have been determined for the reactions of SO4(-) with a series of alkanes and ethers. The tions of SO4(-) with a series of alkanes and ethers. The SO4(-) radical was produced by the laser-flash photolysis of persulfate, S208(-2). For methane, only an upper limit of 1 x 10 to the 6th power l/mol/sec could be determined. For ethane, propane, and 2-methylpropane, rate constants of 0.44, 4.0, and 10.5 x 10 to the 7th power were found. For ethyl and n-propyl ether, rate constants of 1.3 x 10 to the 8th power and 2.2 x 10 to the 8th power l/mol/sec were found and for 1,4-dioxane and tetrahydrofuran, rate constants of 7.2 x 10 to the 7th power and 2.8 x 10 to the 8th power were obtained. The reaction of SO4(-) with allyl alcohol was also studied and found to have a rate constant of 1.4 x 10 to the 9th power l/mol/sec. 10 to the 9th power I/mol/sec.

PB91-203273 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Molecular Physics Div.

Production and Spectroscopy of Small Polyatomic Molecular Ions Isolated in Solid Neon.

Final rept.

M. E. Jacox, and W. E. Thompson. 1990, 10p Sponsored by Army Research Office, Arlington, VA. Pub. in High Temperature Science 28, p225-234 1990.

Keywords: \*Oxygen ions, \*Molecular ions, \*Carbon dioxide, \*Infrared spectra, Molecular structure, Neon, Vibrational states, Reprints, Cluster ions.

The use of a newly developed discharge sampling configuration has led to the stabilization of several small polyatomic molecular ions in solid neon in suffi-cient concentration for detection of their infrared absorptions. The results obtained in these experiments will be illustrated by observations of the ions which appear when carbon dioxide or oxygen is present in the system. In the experiments on carbon dioxide, the the system. In the experiments on carbon dioxide, the antisymmetric stretching absorptions of both CO2(+) and CO2(-) have been identified. An infrared absorption of O4(-) had previously been observed in systems in which an alkali metal atom, M, was codeposited with an Ar-O2 mixture. The appearance of this absorption in the discharge sampling experiments on oxygen defini-tively excludes an alternate assignment of the absorp-tion to an MO4 structure in which two O2 units are coordinated to a central alkali metal atom. Detailed isotopic substitution experiments support the assignment of four infrared absorptions to a vibrational fundamental and combination bands of O4(+) for which no spectroscopic data have previously been reported. Analysis of the spectrum provides information regarding the molecular structure of O4(+).

100,396 PB91-203281 Not available NTIS

Not available NTIS
National Bureau of Standards (NML), Gaithersburg,
MD. Chemical Thermodynamics Div.
Resonance Enhanced Multiphoton Ionization
Spectra of the GeF and GeCl Radicals from 400-500 nm.

Final rept.

R. D. Johnson, J. W. Hudgens, and B. P. Tsai. 1988,

Pub. in Jnl. of Chemical Physics 89, n10 p6064-6068

Keywords: \*Electron transitions, \*Rydberg states, \*Germanium, \*Electron spectra, Electron structure, Energy levels, Excited states, Reprints, \*Germanium fluoride radicals, \*Germanium chloride radicals, \*Multiphoton ionization.

The resonance enhanced multiphoton ionization spectra from 400 to 500 nm of the Germanium chloride and Germanium fluoride radicals are reported.

100,397

PB91-203331 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Molecular Spectroscopy Div.
Molecular Desorption from Solid Surfaces: Laser
Diagnostics and Chemical Dynamics.

Final rept.

D. S. King, and R. R. Cavanagh. 1989, 45p Pub. in Advances in Chemical Physics 76, p45-89

Keywords: \*Surface chemistry, \*Desorption, \*Solids, Spectroscopy, Reviews, Heating, Laser radiation, Nitric oxide, Reprints, Molecular dynamics.

Review of recent state-resolved experiments exploring thermal and laser-driven desorption processes at metal surfaces is presented.

100.398

PB91-203448 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Molecular Spectroscopy Div. Microwave Spectrum and Molecular Structure of the N2-H20 Complex.

Final rept. H. O. Leung, M. D. Marshall, R. D. Suenram, and F. J. Lovas. 1989, 13p

Pub. in Jnl. of Chemical Physics 90, n2 p700-712, 15 Jan 89.

Keywords: \*Complex compounds, \*Water, \*Nitrogen, \*Microwave spectra, \*Molecular structure, Molecular

rotation, Hydrogen bonds, Dipole moments, Nuclear quadrupole resonance, Electron tunneling, Reprints.

The a-type, K = 0 microwave spectrum of the N2-H2O complex has been observed using a pulsed molecular beam Fabry-Perot cavity microwave spectrometer. Seven isotopic species have been studied in the range of 5-23 GHz. The N2-H2O complex exhibits tunnelng motions similar to the 1 -> 2 tunnelling motion of the H2O-DOD complex which gives rise to four components for each rotational transition.

PB91-203471 Not available NTIS National Inst. of Standards and Technology (NML),

Rational History (MML), Gaithersburg, MD. Surface Science Div.

Chemical Effects of Ne+ Bombardment on the MoS2(0001) Surface Studied by High-Resolution Photoelectron Spectroscopy.

Final rept. J. R. Lince, T. B. Stewart, M. M. Hills, P. D. Fleischauer, J. A. Yarmoff, and A. Taleb-Ibrahimi. 1989, 19p

Pub. in Surface Science 210, n3 p387-405 1989.

Keywords: \*Molybdenum disulfide, \*Ion bombard-ment, Photoelectron\_spectroscopy, High resolution, Neon ions, Surfaces, Reprints.

The effect of 1 KeV Ne(1+) ion bombardment on the clean, ordered MoS2(0001) surface was studied using high-resolution photoelectron spectroscopy excited with synchrotron radiation. A qualitative depth distribution of the chemical species present after Ne(1+)bombardment was determined by varying the photon energies employed for core-level spectroscopy. The results indicate that the preferential sputtering of sulfur over molybdenum occurs predominately through a mechanism involving chemical bonding effects, specifically through the preferential emission of polysulfide ions over other species in the bombarded region.

100.400

PB91-203547 Not available NTIS National Bureau of Standards (NML), Gaithersburg,

MD. Chemical Kinetics Div.

Ionic Hydrogen Bonds. Part 1. Thermochemistry,
Structural Implications, and Role in Ion Solvation.

M. Mautner. 1987, 34p See also AD-A178 839.

Pub. in Molecular Structure and Energetics, Chapter 3, v4 p71-104 1987.

Keywords: \*Hydrogen bonds, \*Clustering, \*Solvation, \*lons, Water, Heat of solution, Thermochemistry, Reviews, Molecular structure, Reprints.

The energetics and structural implications of ionic hydrogen bonds are reviewed. Gas-phase clustering properties are compared with solvation in liquid water.

100,401 PB91-203562 Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Quantum Physics Div. Structural Dependence of HF Vibrational Red Shifts in ArnHF, n = 1-4, via High-Resolution Slit Jet

Infrared Spectroscopy.

Final rept.

A. McIroy, R. Lascola, C. M. Lovejoy, and D. J. Nesbitt. 1991, 9p Grant NSF-CHE86-05970

Sponsored by National Science Foundation, Washington, DC. Pub. in Jnl. of Physical Chemistry 95, n7 p2636-2644

Keywords: \*Argon complexes, Van der Waals forces, Supersonic jet flow, Vibrational spectra, Infrared spectroscopy, Hydrogen fluoride, High resolution, Red shift,

The rotationally resolved nu = 1 < 0 HF stretching spectra of Ar(n)Hf, n = 1.4, have been observed by using a slit jet, difference frequency infrared laser spectrometer. The red shift of the HF vibrational frequency is seen to be sensitively dependent on the placement of the Ar with respect to the projection of the HF dipole moment; the largest incremental red shift is observed for the ArHF linear geometry. The n = 1-3 red shifts account for almost half (9.65-19.26/cm) of the shift observed for HF in an Ar matrix (42.4/ cm), suggesting that only the nearest neighbors contribute significantly to the perturbation of the HF vibrational frequency. The geometry of the experimentally observed isomer of Ar4HF places the fourth Ar in what would be the second coordination layer from the HF where it has little effect (<2%) on the observed red shift, supporting the proposed dominance of the near-est neighbors in determining the HF vibrational frequency. In all spectra, no evidence for vibrational predissociation is observed, indicating an extremely long excited state lifetime (approx = or > 16 ns).

100 402

Not available NTIS PR91-203661 National Inst. of Standards and Technology (NML),

Gaithersburg, MD. Chemical Kinetics Div.
Radiolytic Studies of the Redua Reactions of Ruthenium Porphyrins.

Final rept.

S. Mosseri, P. Neta, and P. Hambright. 1989, 5p Pub. in Jnl. of Physical Chemistry 93, n6 p2358-2362

Keywords: \*Ruthenium compounds, \*Porphyrins, \*Oxidation reduction reactions, Radiolysis, Reaction kinetics, Ligands, Cyanides, Reprints.

Oxidation of Ru(II) porphyrins to the Ru(III) and Ru(IV) states and ligand exchange reactions of the various states have been studied by radiolytic methods. RU(II) porphyrins, stabilized with a CO ligand, undergo one electron oxidation on the porphyrin ring to form the piradical cation. When Ru(II)(P)(CO) (P-octaethylporphyrin (OEP) or tetraphenylporphyrin (TPP)) is oxidized by irradiation in CH2CI2, the initial radical cation combines with Cl-, formed by radiolysis of the solvent or added beforehand, with a rate constant of about added beforenand, with a rate constant of about 1000001/mol/s to yield Ru(II)(P+)(CO)(CI-). Irradiation of the same porphyrins in acetonitrile does not result in oxidation but rather in uptake of the CN- produced by the radiolysis to form Ru(III)P(CN-)2. When this produced by the radiolysis to form Ru(III)P(CN-)2. uct is oxidized by irradiation in acetonitrile/CCI(4) solutions, oxidation occurs on the metal center to give Ru(III)P(CN-)2 as the final product. Chemical oxidations and reductions were carried out to complement the radiolysis results.

100.403

PB91-203695 Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Quantum Physics Div. Progress on the Determination of Intermolecular

Potential Energy Surfaces from High Resolution Spectroscopy.

Final rept.

D. J. Nesbitt. 1990, 10p

Grants NSF-CHE86-05970, NSF-PHY86-04504

Sponsored by National Science Foundation, Washing-

Pub. in Dynamics of Polyatomic Van der Waals Complexes, p461-470 1990.

Keywords: \*Complexes, Van der Waals forces, Vibrational states, Infrared spectroscopy, Intermolecular forces, Hydrogen bonds, High resolution, Predissociation, Rare gases, Water, Reprints, \*Potential energy surfaces.

The determination of intermolecular potentials between chemical species has been pursued via a variety of methods including scattering experiments, line broadening, virial coefficients and transport phenom-ena. A powerful alternative approach is to orient the collisional intermediate in a weakly bound complex, and sample the bound region of the potential via high resolution IR spectroscopy on excited intermolecular vibrational states. The author illustrates recent theoretical and experimental progress toward this goal. Molecular systems are discussed that illustrate large amplitude motion characteristic of a (1) 'ball+ball', (2) 'ball+stick', and (3) 'ball+top' intermolecular potential energy surface. The examples are drawn from high resolution near IR measurements on rare gas-hydrospectic and to a construction of the control of the c gen halide and rare gas-water complexes.

100.404

PB91-203703 Not available NTIS

Not available NTIS
National Inst. of Standards and Technology (NML),
Boulder, CO. Quantum Physics Div.
Multiple Intermolecular Bend Vibrational Excitation of a Hydrogen Bond: An Extended Infrared Study of OCOHF.

Final rept. D. J. Nesbitt, and C. M. Lovejoy. 1990, 15p

Grant NSF-CHE86-05970

Sponsored by National Science Foundation, Washing-

# Physical & Theoretical Chemistry

Pub. in Jnl. of Chemical Physics 93, n11 p7716-7730, 1

Keywords: \*Hydrogen bonds, \*Complexes, Near infra-red radiation, Supersonic jet flow, Vibration spectra, Carbon dioxide, Hydrogen fluoride, Laser radiation, Predissociation, Excitation, Bending, Reprints.

The authors report the use of near infrared tunable difference frequency laser absorption methods to investigate low-frequency bending of the intermolecular hydrogen bond in OCOHF complexes. By deliberate thermal warming of the slit jet expansion to 16 K, they observe bending 'hot band' transitions built on the fundamental nu(HF) = <-0 HF stretch from the lowest five internally excited bending states which correspond to low-frequency, skeletal bending of the intermolecular hydrogen bond. In addition, much weaker parallel (delta I = 0) combination band transitions are observed.

100,405 PB91-203760 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Chemical Kinetics Div.

Dissociation Energetics of Simple Diazirines by

Photon and Electron Impact.

H. Okabe. 1987, 14p Pub. in Chemistry of Diazirines, Chapter 7, v2 p19-32

Keywords: \*Dissociation energy, Halohydrocarbons, Absorption spectra, Photolysis, Mass spectra, Heat of formation, Reviews, Thermodynamic properties, Reprints, \*Diazirine, Methyl compounds, Difluorodiazir-

Dissociation energetics by photon and electron impact for six simple diazirines has been reviewed. The data on absorption spectra, UV photolysis, the heats of formation, mass spectra and appearance potentials are presented.

100,406 PB91-203844 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Molecular Spectroscopy Div.

Vibrational, Rotational, and Tunneling Dependence of Vibrational Predissociation in the HF

Dimer.

Final rept. A. S. Pine, and G. T. Fraser. 1988, 8p Pub. in Jnl. of Chemical Physics 89, n11 p6636-6643

Keywords: \*Hydrogen fluoride, \*Predissociation, Vibrational\_spectra, Laser spectroscopy, Line width, Dimers, Reprints.

Vibrational predissociation linewidths have been resolved in the two H-F stretching bands of the HF dimer using an optothermal (bolometer-detected) molecularbeam color-center laser spectrometer. In addition to the strong vibrational mode dependence reported earlier by several groups, one observes a substantial K-rotational and tunneling dependence to the longerlived mode, nu(1), which is associated with the 'free-H' stretch. The predissociation linewidths (FWHM in MHz) for this vibration are 6.4(5) for K=0(+), 9.5(5)for K=0(-), 10.2(5) for K=1(+) and 11.8(5) for K=(-), where the +/- superscripts refer to the symmetric/ antisymmetric tunneling states. The K=0 levels of the 'bound-H' stretch have tunneling-independent widths of 330(30) MHz. Extraneous broadening due to saturation effects was observed and corrected for in these measurements.

100,407 PB91-203927 Not available NTIS National Inst. of Standards and Technology (CSTL), Gaithersburg, MD. Biotechnology Div.
Frequency Dependence of Catalyzed Reactions in a Weak Oscillating Field.

Final rept.

B. Robertson, and R. D. Astumian. 1991, 6p Pub. in Jnl. of Chemical Physics 94, n11 p7414-7419, 1

Keywords: \*Reaction kinetics, \*Catalysis, \*Frequency response, \*Mathematical models, Ion mobility, Phosphatases, Erythrocytes, Reprints, \*Lorentz curves, \*Oscillating fields, Sodium/potassium adenosine tri-

The frequency dependence of the average rates of reactions catalyzed by one or more catalysts in a weak oscillating field is derived. The average rates are sums of Lorentzian curves whose characteristic frequencies the inverse relaxation times of the normal modes of the kinetic system and whose amplitudes are quadratic in the field. The signs of the Lorentz amplitudes can be either positive or negative, so the rates versus frequency can have a variety of shapes, including frequency windows. One can get relaxation times and amplitudes by measuring steady-state rates as a func-tion of the frequency of the field. The theory is applied to determine the Lorentz amplitudes and characteristic frequencies of ion transport rates catalyzed by Na(+)-K(+)ATPase in erythrocytes.

100,408 PB91-204008 Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Quantum Physics Div. High-Resolution Infrared Flash Kinetic Spectros-

copy of OH Radicals.

A. Schiffman, D. D. Nelson, M. S. Robinson, and D. J. Nesbitt. 1991, 8p Contract AFOSR-F49620-86-C-0056

Sponsored by Air Force Office of Scientific Research, Bolling AFB, DC.

Pub. in Jnl. of Physical Chemistry 95, n7 p2629-2636

Keywords: \*Hydroxyl radicals, \*Reaction kinetics, \*Ethane, \*Butanes, \*Propane, Infrared lasers, Infrared spectra, Photolysis, Atmospheric circulation, Reprints, Flash kinetic spectroscopy.

A high-resolution infrared flash kinetic spectrometer is used for time- and frequency-resolved studies of the OH radical. OH is produced by 193-nm excimer laser photolysis of HNO3/buffer gas mixtures in a 100-cm flow tube and is probed via weak fractional absorption of light from a widely tunable (2.35-3.59 micrometers) permit determination of absolute OH number densities. The spectrometer is used to measure rate constants for the reactions of OH with ethane (k1), propane (k2), n-butane (k3), and isobutane (k4). The reliability of these measurements is tested on a variety of rotational, spin-orbit, and lambda-doublet states, with several buffer gases, and over more than an order of magnitude of alkane concentrations. The resulting rate constants are, in units of 10 to the -12th power cc/molecule/sec, k1 = 0.243 + or - 0.012, k2 = 1.02 + or - 0.05, k3 = 2.35 + or - 0.08, and k4 = 2.11 + or - 0.09. The rate constants for the ethane, n-butane, and isobutane reactions agree with some previous deter-minations but are found to be between 10% and 25% lower than values currently used in atmospheric mod-eling; it is recommended that these values be revised to reflect the lower rates from the study. Current models of atmospheric air flow based on these rate constants, as well as those of previously accepted values, are found to be inconsistent with daily changes in observed atmospheric alkane concentrations.

Not available NTIS PB91-204024 National Inst. of Standards and Technology (NML), Roulder, CO. Quantum Physics Div.
Investigation of Internal Rotor Dynamics of NeDCl and ArDCl via Infrared Absorption Spectroscopy.

Final rept.

M. Schuder, D. Nelson, and D. J. Nesbitt. 1991, 16p Grants NSF-CHE86-05970, NSF-PHY86-04504 Sponsored by National Science Foundation, Washing-Pub. in Jnl. of Chemical Physics 94, n9 p5796-5811, 1

May 91.

Keywords: \*Argon complexes, \*Neon complexes, Van der Waals forces, Supersonic jet flow, Intermediate in-frared radiation, Laser radiation, Vibrational spectra, Deuterium compounds, Hydrogen chloride, Infrared spectroscopy, Predissociation, Reprints, Potential energy surfaces.

The van der Waals complexes, NeDCI and ArDCI, are produced in a slit jet supersonic expansion and observed via direct absorption of funable mid-infrared Pb-salt diode laser radiation. The relative fundamental vs bend combination band intensity distributions are very different for the two complexes. The ArDCI fundamental to Pi bend combination band intensity ratio is 4:1, whereas for NeDCl the corresponding ratio is 1:8. This anomalous intensity pattern for NeDCl and the proxim-

ity of the bend combination bands to the DCI R(0) line indicate that the DCI diatomic is exhibiting nearly free rotation within the complex, compared to more restricted librational motion of DCI in ArDCI. Experimentally determined rotational constants, vibrational frequencies, and relative intensities are compared to predictions based on existing empirical potential surfaces.

100,410

PB91-204065
Not available NTIS
National Inst. of Standards and Technology (NEL),
Gaithersburg, MD. Thermophysics Div.

Thermodynamic Properties of Aqueous Solutions at High Temperatures; Needs, Methods, and Challenges.

J. M. H. Levelt Sengers. 1990, 17p Pub. in International Jnl. of Thermophysics 11, n2

Keywords: \*Aqueous solutions, \*Thermodynamic properties, \*Thermophysical properties, \*Hydrothermal systems, Autoclaves, Debye-Huckel theory, High temperature tests, High pressure tests, Data bases, Methodology, Reviews, Hot-water systems, BWR type reactors, Hydroelectric power, Reprints, Research needs

Needs exist for thermophysical data on aqueous solu-tions at high temperatures and pressures in many dif-ferent areas of science and engineering. These needs are reviewed and references are given to recent relevant conference proceedings, reviews and papers. Aspects and drawbacks are discussed of current methods, which are most often extensions to high temperatures of methods developed for liquid water. The challenges posed by engineering needs and by new phenomena resulting from experimental breakthroughs are discussed. Some examples are given of alternative approaches more suitable for highly compressible media.

100 411 PB91-216713

(Order as PB91-216705, PC A07/MF A01) National Inst. of Standards and Technology, Boulder,

High-Temperature Transient Hot-wire Thermal Conductivity Apparatus for Fluids.
R. A. Perkins, H. M. Roder, and C. A. Nieto de Castro. 1991, 23p

Prepared in cooperation with Lisbon Univ. (Portugal). Dept. de Quimica.

Included in Jnl. of Research of the National Institute of Standards and Technology, v96 n3 p247-269 May/Jun

Keywords: \*Thermal conductivity, \*Thermal diffusivity, Measuring instruments, Hot-wire gages, Specific heat, High temperature, Toluene, Nitrogen, Argon, Fluids.

A new apparatus for measuring both the thermal conductivity and thermal diffusivity of fluids at tempera-tures from 220 to 775 K at pressures to 70 MPa is de-scribed. The instrument is based on the step-powerforced transient hot-wire technique. Performance of the instrument was verified with measurements on liquid toluene as well as argon and nitrogen gas. In particular, new data for the thermal conductivity of liquid toluene near the saturation line, between 298 and 550 K, are presented. These new data can be used to illustrate the importance of radiative heat transfer in transient hot-wire measurements. Thermal conductivity data for liquid toluene, which are corrected for radi-ation, are reported. From the measured thermal conductivity and thermal diffusivity, the authors can calculate the specific heat, Cp, of the fluid, provided that the density is measured, or available through an equation of state.

100,412

PB91-236521 Not available NTIS National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Office of Intelligent Processing of

Problem of Detailed Balance and Model Line-shapes in Collision-Induced Rotovibrational Bands: H2-H2 and H2-He.

Final rept.

G. Birnbaum, and A. Borysow. 1991, 12p Pub. in Molecular Physics 73, n1 p57-68 1991.

Keywords: \*Molecular collisions, Vibrational spectra, Hydrogen, Helium, Line shape, Reprints.

When account is taken of the vibrational dependence of the potential function, the usual condition of detailed balance taken with respect to the vibrational-rotational frequencies does not apply, and model spectral functions satisfying the condition are inaccurate. A model correlation function is derived that deals with the case of vibration-dependent potentials. The parameters of the model are computed from relations involving the spectral moments. The model is shown to give spectral shapes, for a number of examples involving the fundamental and first overtone bands of H2-He and H2-H2 at room temperature and 1000K, in excellent agreement with spectra calculated quantum mechanically from first principles. The model is useful for predicting the collision-induced vibrational spectra for these and other systems for which the vibration-de-pendent induced dipole and potential are known.

#### 100.413

PB91-236547 Not available NTIS National Inst. of Standards and Technology (CSTL), Gaithersburg, MD. Surface and Microanalysis Science

Photodissociation Dynamics of Mo(CO)6 at 266 nm and 355 nm: CO Photofragment Kinetic-Energy and Internal-State Distributions.

Final rept.

S. A. Buntin, R. R. Cavanagh, L. J. Richter, and D. S. King. 1991, 14p

Sponsored by Department of Energy, Washington, DC. Pub. in Jnl. of Chemical Physics 94, n12 p7937-7950, 15 Jun 91.

Keywords: \*Carbon monoxide, \*Photodissociation, Near ultraviolet radiation, Photofragment spectroscopy, Laser induced fluorescence, Kinetic energy, Photolysis, Reprints, \*Hexacarbonylmolybdenum.

The internal-state and kinetic-energy distributions of the CO photofragments from the 266 and 355 nm pho-tolysis of Mo(CO)6 have been measured under collision-free conditions using vacuum-ultraviolet laser-in-duced fluorescence. The Doppler-broadened CO photofragment line shapes indicate that the translational energy distributions are isotropic and Maxwellian. There is no photolysis-laser wavelength or internalstate dependence to the extracted translational 'temperatures.' The observed energy partitioning and kinetic-energy distributions are inconsistent with an impulsive ejection of a single CO ligand. The results also suggest that the photodissociation of Mo(CO)6 at 266 and 355 nm involves a common initial 'state' and that similar exit channel effects are operative.

### 100,414

PB91-236570 Not available NTIS National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Polymers Div.

Temperature Gradient in Differential Scanning Calorimetry.

Final rept.

S. S. Chang. 1991, 7p

Pub. in Thermochimica Acta 178, p195-201 1991.

Keywords: \*Calorimeters, \*Heat measurement, \*Thermal analysis, \*Temperature gradients, Reaction heat, Heat flow, Dynamic tests, Measurement, Epoxy resins, Mathematical models, Curing, Reprints.

A temperature gradient is required for any type of heat flow process. In a dynamic calorimeter, temperature gradients exist in the entire calorimetric system during the measurement of temperature differences or heat flow. Most organic materials are of relatively low thermal conductivity in comparison to metallic and inor-ganic materials. Therefore large temperature gradients are expected to exist in organic materials during the measurement. The magnitude of the temperature gradient can be estimated through a simple modeling procedure. The results of experimentally determined temperature gradients during the cure of an epoxy resin in a differential scanning calorimeter are presented to confirm the expected magnitude of temperature nonuniformity.

### 100.415

PR91-236661 Not available NTIS National Inst. of Standards and Technology (PL), Gaithersburg, MD. Molecular Physics Div. Rotational Spectrum and Structure of the Complex Ar-Ch3CN.

Final rept.

R. S. Ford, R. D. Suenram, G. T. Fraser, F. J. Lovas, and K. R. Leopold. 1991, 7p Grant NSF-CHE88-07895

Sponsored by National Science Foundation, Washing-

Pub. in Jnl. of Chemical Physics 94, n8 p5306-5312, 15 Apr 91.

Keywords: \*Argon complexes, \*Acetonitrile, Van der Waals forces, Microwave spectra, Molecular structure, Reprints.

The microwave spectrum of the weakly bound complex Ar-CH3CN has been observed using a pulsednozzle Fourier-transform microwave spectrometer. The spectrum is characteristic of an asymmetric rotor with nearly free internal rotation of the methyl group. Spectroscopic constants for the ground internal rotor state, in megaHertz, are given. The complex has a T-shaped geometry in which the acetonitrile axis is nearly perpendicular to the line joining the centers of mass of the monomers, and the methyl group undergoes nearly free internal rotation. The center-of-mass separation is 3.6505(7) A and the dipole moment component along the b inertial axis of the complex is 3.802(5) D. The latter is quantitatively accounted for by the sum of the monomer permanent moment and the dipole-induced dipole in the argon.

100.416 PB91-236679 Not available NTIS National Inst. of Standards and Technology (PL), Gaithersburg, MD. Molecular Physics Div. Optothermal-Detected Microwave-Sideband CO2-Laser Spectroscopy of Ar-NH3.

G. T. Fraser, A. S. Pine, and W. A. Kreiner. 1991, 7p Pub. in Jnl. of Chemical Physics 94, n11 p7061-7067, 1

Keywords: \*Argon complexes, \*Ammonia, Intermolecular forces, Van der Waals forces, Laser spectroscopy, Carbon dioxide lasers, Infrared spectra, Reprints.

A microwave-sideband CO2-laser optothermal spectrometer with a resolution better than 1 MHz has been used to record the infrared spectrum of Ar-NH3 in the vicinity of the aR(O,O) line of the nu(2) vibration of free NH3. A Pi < - Sigma type band is observed, giving a positive I-type doubling constant q, of 90.9 MHz for the upper state. The nu(2) vibrationally excited complex is found to predissociate in less than the 0.9 ms transit time between the bolometer detector and laser-excitation region. A lower limit to the upper-state lifetime can be obtained from the observed linewidths, which range from 1.5 to 3 MHz (FWHM). The present results agree with and extend the previous free-jet diode-laser absorption measurements on this band.

PB91-236737 Not available NTIS Not available NTS
National Inst. of Standards and Technology (PL),
Gaithersburg, MD. Molecular Physics Div.
Van der Waals Complexes in 1,3-Dipolar Cycloaddition Reactions: Ozone-Ethylene.

C. W. Gillies, J. Z. Gillies, R. D. Suenram, F. J. Lovas, E. Kraka, and D. Cremer. 1991, 10p Pub. in Jnl. of the American Chemical Society 113, n7

Keywords: \*Oxygen complexes, \*Ozone, \*Ethylene, Van der Waals forces, Rotational spectra, Microwave spectra, Electric dipole moments, Deuterium compounds, Molecular structure, Cyclization, Reprints

Microwave spectra of O3-CH2=CH2, O3-CD2=CH2, O3-trans-CHD=CHD, and O3-cis-CHD=CHD have been observed with a pulsed-beam Fabry-Perot cavity, Fourier transform microwave spectrometer. Internal motion in the van der Waals complex give two states for the normal, 1,1-dideuterated and trans-1,2-dideuterated isotopic forms. The c-type transitions of the two states for the isotopic species above, as well as the one observed isotopic form of O3-cis-CHD=CHD, independently fit to an asymmetric top Watson Hamiltonian. Stark effect measurements were performed.

Not available NTIS PB91-236778 National Inst. of Standards and Technology (CSTL), Gaithersburg, MD. Thermophysics Div. Phase Equilibria and Critical Lines in Model Water/ Salt Mixtures.

Final rept.

A. H. Harvey. 1991, 6p Pub. in Jnl. of Chemical Physics 95, n1 p479-484, 1 Jul

Keywords: \*Solutions, \*Aqueous electrolytes, \*Mathematical models, \*Phase diagrams, \*Thermodynamics equilibrium, \*Critical point, Thermodynamics, Dipoles, Spheres, Binary mixtures, Reprints, \*Critical lines, \*Mean spherical approximation.

The mean spherical approximation solution for the thermodynamics of a mixture of equal-sized dipolar hard spheres and charged hard spheres is used to calculate phase equilibria and critical lines. The binary system is characterized by the dimensionless ratio of the dipolar strength to the strength of the charges. At high values of this ratio, the critical curve is interrupted by a liquid-liquid equilibrium and the phase diagram (under the usual classification scheme) is type III. As the ratio is lowered, the critical curve becomes contin-uous; this is type I or II behavior. The continuous critical line is maintained until the critical temperature of the ionic component exceeds that of the dipolar component by a factor of approximately 3.56; such a lengthy unbroken critical line is unusual in ordinary fluid systems but is observed in many mixtures of water with strong electrolytes. At sufficiently low values of the dimensionless ratio, the critical line is interrupted very near the critical point of the dipolar component; these systems exhibit type IV or V behavior. The simple model used here reproduces the qualitative features of the phase diagrams of real water/salt systems. Insights from the model suggest at least partial explanations for the unusually long unbroken critical lines observed in many of these systems.

100,419 PB91-236836 Not available NTIS National Inst. of Standards and Technology (PL), Vibrational Spectra of Molecular lons Isolated in

Solid Neon, 6, CO4(1-). Final rept.

M. E. Jacox, and W. E. Thompson. 1991, 7p

See also PB91-149906. Pub. in Jnl. of Physical Chemistry 95, n7 p2781-2787, 4

Apr 91.

Keywords: \*Neon, \*Matrix isolation, \*Molecular ions, Vibrational spectra, Infrared spectra, Cryogenics, Carbon dioxide, Oxygen, Molecular structure, Reprints, \*Percarbonate ion, Force constants.

When a Ne:CO2:O2=200:1:1 mixture is codeposited at approximately 5 K with a beam of neon atoms that have been excited in a microwave discharge, several prominent infrared absorptions appear in the resulting deposit. In addition to the absorptions of unreacted CO2, absorptions previously assigned to O4(1+) and O4(1-) are present, and new absorptions appear at 697, 1256, 1865, and 1895 cm-1. Detailed isotopic substitution experiments demonstrate that these new absorptions are contributed by a product of formula CO4 in which the CO2 moiety is joined to O2 in such a way that the two O atoms of each of these groups are nonequivalent. Arguments are presented indicating that this product is the C04(1-) anion. The infrared frequencies of the isotopically substituted species have been used for a least-squares force constant adjustment calculation, assuming a planar O2CdashO2(1-) C(s) structure in which most of the negative charge remains on the O2 moiety. The photodestruction threshold of CO4(-) lies near 260 nm. Evidence has been obtained for the formation of CO3(1-) or of CO(3) in an excited cate with 2 feet or most of the control of CO3(1) or of CO(3) in an excited cate with 2 feet or most of the control of CO3(1-) or of CO(3) in an excited cate with 2 feet or most of control of CO3(1-) or of CO(3) in an excited cate with 2 feet or most of control of CO3(1-) or of CO(3) in an excited cate with 2 feet or most of control of CO3(1-) or of CO(3) in an excited cate with 2 feet or most of control of CO3(1-) or of CO(3) in an excited cate with 2 feet or of CO3(1-) or of CO(3) in an excited cate with 2 feet or of CO3(1-) or of CO(3) in an excited cate with 2 feet or of CO3(1-) or of CO(3) in an excited cate with 2 feet or of CO3(1-) or of CO(3) in an excited cate with 2 feet or of CO3(1-) or of CO(3) in an excited cate with 2 feet or of CO3(1-) or of CO(3) in an excited cate with 2 feet or of CO3(1-) or of CO(3) in an excited cate with 2 feet or of CO3(1-) or of CO(3) in an excited cate with 2 feet or of CO3(1-) or of CO(3) in an excited cate with 2 feet or of CO3(1-) or of CO(3) in an excited cate with 2 feet or of CO3(1-) or of CO(3) in an excited cate with 2 feet or of CO3(1-) or of CO(3) in an excited cate with 2 feet or of CO3(1-) or of CO(3) in an excited cate with 2 feet or of CO3(1-) or of CO(3) in an excited cate with 2 feet or of CO3(1-) or of CO(3) in an excited cate with 2 feet or of CO3(1-) or of CO3(1excited state with 3-fold symmetry, for which randomization of the oxygen isotopic substitution occurs.

100.420 PB91-236851 Not available NTIS National Inst. of Standards and Technology, Gaithers-

Temperature Measurements in Flames Using Thermally Assisted Laser-Induced Fluorescence of Ga.

Final rept. R. Joklik, J. Horvath, and H. Semerjian. 1991, 8p. Contract N0001989IPB7387

Sponsored by Naval Air Systems Command, Washing-

Pub. in Applied Optics 30, n12 p1497-1504, 20 Apr 91. Keywords: \*Temperature measurement, \*Flames, Laser induced fluorescence, Gallium, Reprints.

# Physical & Theoretical Chemistry

The use of thermally assisted fluorescence (THAF) for temperature measurements has been investigated in a laminar, premixed C2H2/O2/Ar flame seeded with Ga atoms. Average temperature measurements were made with an uncertainty of less than + or - 100 K in flames > 2150 K and were found to be in agreement with sodium line reversal temperature measurements and equilibrium calculations. In both fuel rich and lean flames spanning equivalence ratios from 0.75 to 2.0, it was found that composition influenced the measured temperatures, resulting in an accuracy of + or - 100 K over the range of flame conditions. Results indicate that THAF with gallium as the thermometric species is limited to cases in which an inefficient quencher, such as a rare gas, is the primary diluent.

100,421 PB91-236869

Not available NTIS National Inst. of Standards and Technology (PL), Gaithersburg, MD. Molecular Physics Div. Molecular-Beam Optothermal Spectroscopy of the

9.6 mum nu14.

Final rept.

M. L. Junttila, J. L. Domenech, G. T. Fraser, and A.

Sponsored by National Aeronautics and Space Administration, Washington, DC. Pub. in Jnl. of Molecular Spectroscopy 147, p513-520

Keywords: \*Benzene, Intermediate infrared radiation, Carbon dioxide lasers, Infrared spectra, Ground state, Molecular beams, Reprints.

The nu(sub 14) e(sub 1u)-symmetry fundamental band of C(6)H(6) has been recorded with sub-Doppler resolution under collisionless low-temperature molecularbeam conditions using bolometric detection of mole-cules excited by tunable microwave sidebands of a Lamb-dip-stabilized CO2 laser. The sidebands cover about 40% of the spectrum between laser lines in which 117 transitions for J,  $K=\sigma < 11$  have been observed and fit to a precision of  $+\sigma - 24$  kHz, yielding improved ground and excited state rotational constants with nearly microwave accuracy. The authors' measured ground state rotational constant, B(sub 0)=0.18977389(3)/cm, is compared with several disparate values reported previously.

100,422 PB91-236885 Not available NTIS National Inst. of Standards and Technology (MSEL),

Gaithersburg, MD. Polymers Div.
Temperature Dependence of Probe Diffusion in **Bulk Polymer Matrices.** 

Final rept

H. Kim, D. Waldow, C. Han, Q. Tran-Cong, and M. Yamamoto. 1991, 5p Pub. in Polymer Communications 32, n4 p108-112

Keywords: \*Polymerization, \*Diffusion, \*Rayleigh scattering, \*Probes, Chemical radiation effects, Predictions, Matrix materials, Temperature dependence, Photochemical reactions, Melts, Measurement, Dimers, Reprints, Cyclophane.

The temperature dependence of the diffusion coefficients for a photobleachable molecular probe in various polymer matrices has been studied using forced Rayleigh scattering (FRS). The probe molecule, a cyclophane derivative, is demonstrated to be a suitable probe for the FRS experiment due to the characteristics of the photodimerization reaction. The dynamic range of the FRS experiment enabled the measurement of the self diffusion coefficients over a range of nearly eight orders of magnitude. The temperature de-pendence of the self diffusion coefficients is well deperiodice of the self-diffusion coefficients is well described by the Williams, Landel, Ferry (WLF) equation for all the polymer matrices studied. In addition, the data from the individual polymer matrices can be shifted to construct a universal curve which is also well described by the WLF equation.

PB91-236984 Not available NTIS National Inst. of Standards and Technology (NML),

Boulder, CO. Time and Frequency Div.
Heterodyne Frequency Measurements of CO and OCS Beyond 2100 cm(-1).

A. G. Maki, J. S. Wells, and D. A. Jennings. 1990, 6p Sponsored by National Aeronautics and Space Admin-istration, Washington, DC. Office of Atmospheric Re-

Pub. in Jnl. of Molecular Spectroscopy 144, p224-229

Keywords: \*Carbon dioxide, \*Molecular spectra, \*Infrared spectra, \*Carbon oxysulfide, Frequencies, Tables(Data), Band spectra, Lasers, Reprints.

Infrared heterodyne frequency measurements are given for absorption lines of the 04(o)0-00(o)0 band of OCS and the fundamental band of CO. Transition frequencies of several isotopomers of CO are given. The frequency measurements were based on doubled CO2 laser radiation used as a local oscillator and as a frequency standard. Tables of wavenumber standards based on both OCS and CO absorption lines are given.

PB91-237016 Not available NTIS National Inst. of Standards and Technology (PL), Gaithersburg, MD. Molecular Physics Div.

Perpendicular Bands of Cyclopropane in the 3.5mum Region.

Final rept.

D. W. Merdes, J. Pliva, and A. S. Pine. 1991, 17p Pub. in Jnl. of Molecular Spectroscopy 147, p431-447

Keywords: \*Cyclopropane, \*Infrared spectra, Intermediate infrared radiation, Laser spectroscopy, Band spectra, High resolution, Reprints.

The spectrum of the cyclopropane molecule was measured in the region 2898.5 to 3157.3/cm with Doppler-limited resolution using a difference frequency laser spectrometer. Deconvolution was used to further enhance the effective resolution in the main part of the highly perturbed spectrum. The region below about 3060/cm contains perpendicular bands. The nu(2) + nu(9)E' state is also perturbed by anharmonic interactions with additional E' states. A comprehensive analysis of this complex system of perpendicular bands based on a Hamiltonian model of the main interactions yielded much improved spectroscopic constants, as well as information on seven tentatively identified perturbing states.

100.425

PB91-237032 Not available NTIS National Inst. of Standards and Technology (CSTL), Gaithersburg, MD. Surface and Microanalysis Science

Direct Detection of Atom Vaporization by Laser Resonance Ionization as a Probe of Gas-Surface Chemisorption Mechanisms.

Final rept. M. H. Mintz, P. Shuker, and J. Fine. 1990, 5p
Pub. in Surface Science Letters 238, pL473-L477

Keywords: \*Chemisorption, \*Surface chemistry, \*Metals, \*Laser spectroscopy, Mechanism, Low temperature, Ambient temperature, Oxygen, Magnesium, Polycrystals, Measurement, Laser heating, Vaporizing, Reprints, Laser resonance ionization.

A new method for monitoring the development of chemisorption processes on metallic surfaces (either single crystals or polycrystalline), is demonstrated. The method involves direct detection of metal vaporization by laser resonance ionization. It has a remarkably high sensitivity and selectivity for detecting vapor densities (of the order of a few atoms cm/cc) enabling vaporization measurements even at relatively low temperatures (about room temperature). The method is demonstrated for the case of room-temperature chemisorption of oxygen on polycrystalline magnesium. A random initial chemisorption stage followed by an island growth stage is seen to dominate the chemisorption process.

100,426

PB91-237149 Not available NTIS National Bureau of Standards (NEL), Boulder, CO. Chemical Engineering Science Div.

Mass Transfer Coefficients in Two-Phase Aqueous

Extraction.

Extraction.
Final rept.
T. A. Patil, S. K. Sikdar, S. B. Sawant, and J. B. Joshi. 1988, 6p
Pub. in Chemical Engineering Jnl. and Biochemical Engineering Jnl. 39, n1 pB1-B6 1988.

Keywords: \*Mass transfer, Bovine serum albumin, pH, Temperature, Molecular weight, Polyoxyethylene, Separation, Extraction, Reprints.

Mass transfer coefficients of bovine serum albumin in two-phase aqueous systems were measured in a 51 mm i.d. stirred cell with a plane interface. Two systems, sodium sulfate-PEG and dextran-PEG were employed. The effects of stirring speed, pH, temperature and the PEG molecular mass on mass transfer and partition coefficients were investigated. The authors strong dependence of mass transfer and partition on pH. Using the variation of the overall mass transfer coefficients with pH, the authors were able to determine the individual-phase mass transfer coefficients.

100.427

PB91-237164 Not available NTIS National Inst. of Standards and Technology (PL), Gaithersburg, MD. Ionizing Radiation Div. Molecular-Orbital Studies via Satellite-Free X-ray

Fluorescence: CI K Absorption and K-Valence-Level Emission Spectra of Chlorofluoromethanes. Final rept.

Final rept.
R. C. C. Perera, P. L. Cowan, D. W. Lindle, R. E. LaVilla, T. Jach, and R. D. Deslattes, 1991, 10p Sponsored by Department of Energy, Washington, DC. Pub. in Physical Review A 43, p3609-3618 1991.

Keywords: \*Dichlorodifluoromethane, \*Chloromethanes, X ray fluorescence, X ray absorption, Synchro-tron radiation, Molecular orbitals, Reprints, \*Chlorotrifluoromethane.

X-ray absorption and emission measurements in the vicinity of the chlorine K edge of the three chlorofluoromethanes have been made using monochromatic synchrotron radiation as the source of excitation. By selectively tuning the incident radiation to just above the Cl is single-electron ionization threshold for each molecule, less complex x-ray-emission spectra are obtained. This reduction in complexity is attributed to the elimination of multielectron transitions in the CI K shell, which commonly produce satellite features in x-ray emission. The resulting 'satellite-free' x-ray-emission spectra exhibit peaks due only to electrons in valence molecular orbitals filling a single CI is vacancy. These simplified emission spectra and the associated x-ray absorption spectra are modeled using straightforward procedures and compared with semiempirical ground-state molecular-orbital calculations. Good agreement is observed between the present experimental and theoretical results for valence-orbital energies and those obtained from ultraviolet photoemission, and between relative radiative yields determined both experimentally and theoretically in the work.

100,428

PB91-237172 Not available NTIS Not available N IS
National Inst. of Standards and Technology (PL),
Gaithersburg, MD. Molecular Physics Div.
Hydration of Carbon Dioxide: The Structure of
H2O-H2O-CO2 from Microwave Spectroscopy.

Final rept.

K. I. Peterson, R. D. Suenram, and F. J. Lovas. 1991. Pub. in Jnl. of Chemical Physics 94, n1 p106-117, 1

Jan 91.

Keywords: \*Carbon dioxide, \*Hydration, Electric dipole moments, Molecular structure, Molecular spectra, Rotational spectra, Hydrogen bonds, Complexes, Trimers, Water, Reprints.

The structure of the gas-phase trimeric complex H2O-H2O-CO2 is determined through an analysis of the rotational spectra of ten isotopically substituted species. These spectra were measured in the region between 7.5 and 18 GHz using a pulsed-molecular-beam Fourier-transform microwave spectrometer. The structure is found to be cyclical with the dimer-type bond lengths within the trimer being approximately the same as those found in the free heterodimers. One water molecule is oxygen bound to the carbon atom of the CO2 and is also hydrogen bonded to the oxygen of the second water molecule. The second water molecule is in turn hydrogen bonded to one of the oxygens of the CO2 molecule. The observed splittings are most likely due to a hydrogen-exchanging internal rotation of the second water molecule.

100.429

PB91-237487 Not available NTIS National Inst. of Standards and Technology (PL), Gaithersburg, MD. Molecular Physics Div.

Microwave Spectra and Electric Dipole Moments of X(4)Sigma(1-)1/2 VO and NbO. Final rept.

R. D. Suenram, G. T. Fraser, F. J. Lovas, and C. W.

Gillies. 1991, 9p Pub. in Jnl. of Molecular Spectroscopy 148, p114-122

Keywords: \*Niobium oxides, \*Vanadium oxides, \*Electric dipole moments, Microwave spectra, Rotational spectra, Fourier transform spectrometers, Reprints.

Microwave spectra and electric dipole moments have been measured for the X(sup 4)Sigma(sub 1/2, sup -) states of VO and NbO using a pulsed-nozzle Fouriertransform microwave spectrometer with a laser-vaporiation source. An analysis of the Stark effect of hyper-fine components of the J=3/2<-1/2 transition yields dipole moments of 3.355(14) and 3.498(7)D for VO and NbO, respectively. The dipole-moment meas-terments are composed with speech in idia. urements are compared with recent ab initio calcula-

100,430 PB91-237529 Not available NTIS National Inst. of Standards and Technology (CSTL), Gaithersburg, MD. Chemical Kinetics and Thermodynamics Div.

Stabilities of Substituted Benzyl Radicals: Dissociation Rates of Aminoethylbenzenes, Hydroxyethylbenzenes, and Cyanoethylbenzenes. Final rept. M. M. Suryan, and S. E. Stein. 1989, 4p

Pub. in Jnl. of Physical Chemistry 93, n21 p7362-7365

Keywords: \*Reaction kinetics, \*Dissociation, \*Chemical stability, Decomposition reactions, Pyrolysis, Low pressure research. Free radicals, Chemical bonds, Reprints, \*Benzyl radicals, Benzene/aminoethyl, Benzene/hydroxyethyl, Benzene/cyanoethyl.

Rates of unimolecular thermal decomposition of amino, hydroxy, and cyano ethylbenzenes have been determined by the very low pressure pyrolysis technique. These rates relative to the rate of dissociation of ethylbenzene, yield the following substituent effects on benzylic C-C bond strengths: NH2 (ortho)-2.7, (meta)-0.3, and (para)-1.7; OH (ortho)-1.7, (meta)-0.7, and (para)-1.1; CN (ortho)-0.3, (meta)0.4, and (para)-1.5. These effects are generally smaller than those for substituted propers and follow effects and the control of the contr stituted anisoles and follow different trends. Along with results of ESR studies of Nicholas and Arnold, the present substituent effects indicate that a 1 G change in the benzylic hyperfine coupling constant corresponds to a 1.8 kcal/mol change in bond strengths.

PB91-237537 Not available NTIS National Inst. of Standards and Technology (CSTL), Gaithersburg, MD. Chemical Kinetics and Thermodynamics Div

Dissoclation of Substituted Anisoles: Substituent Effects on Bond Strengths.

Final rept. M. M. Suryan, S. E. Stein, and S. A. Kafafi. 1989, 7p Pub. in Jnl. of the American Chemical Society 111, n13

p4594-4600 1989.

Keywords: \*Anisoles, \*Dissociation, \*Molecular structure, Chemical bonds, Aryl ethers, Free radicals, Reaction kinetics, Reprints, \*Bond strength, \*Substituent

Rates of O-methyl homolysis of 24 substituted anisoles were determined by the very-low-pressure pyrolysis technique. All ortho substituents weakened the Omethyl bond, with effects ranging from -0.2 to -7.4 kcal. Effects of para substituents varied over the narrowerrange 1.2 to -2.9 kcal, while in the meta position effects were even smaller (1.1 to -1.0 kcal, including substituents previously studied). There was some correlation between the measured differences in substituent effects on bond strengths (DeltaBDE) and literature rates of H-abstraction from substituted phenols, but differences were also clear, presumably reflecting polar effects in the abstraction reactions. Overall, DeltaBDE showed a fair correlation with the substituent constant (sc) (cor. coeff. = 0.91). Deviations were attributed to contributions to sc from substituent bond dipole-charge interaction. A good correlation was also found between DeltaBDE and ESR hyperfine coupling constants (hfcc) for o- and p-substituted phenoxy radicals. However, substituents affected the degree of apparent spin density alternation in the ring rather than absolute values, obscuring the physical connection between DeltaBDE and hfcc.

100.432

PB91-237636 Not available NTIS National Bureau of Standards (IMSE), Gaithersburg, MD. Reactor Radiation Div.

Neutron Spectroscopic Evidence for Adsorbed

Hydroxyl Species on Platinum Black. Final rept.

T. J. Udovic, J. J. Rush, and R. R. Cavanagh. 1988,

Pub. in Jnl. of the American Chemical Society 110, n16 p5590-5591 1988.

Keywords: \*Platinum black, \*Catalysts, \*Adsorption, \*Surface chemistry, \*Hydroxyl compounds, Neutron scattering, Monomolecular films, Hydrogen, Vibration-al spectra, Spectrum analysis, Volumetric analysis, Chemical reactions, Synthesis(Chemistry), Oxygen, Reprints, Electron energy loss spectroscopy.

The scarcity of vibrational spectroscopic studies confirming the stability of hydroxyl species on high-surface-area metallic materials has led to the use of incoherent inelastic neutron scattering (IINS) to investigate the possible extent of surface hydroxyl formation from the reaction of oxygen with hydrogen on platinum black. The titration of 0.4 monolayers residual H on the reduced Pt black surface with 02 (O:H = 1) at 80K followed by equilibration at 300K and recooling to 80K led to the disappearance of residual hydrogen vibrational peaks at 104 and 152 meV and the formation of a vibrational peak maximized at 128 meV. The peak became more intense upon the further addition of equimolar amounts of H2 and O2 (ca. 0.5 more monolayers each of O and H) to the Pt surface at 80K followed by similar 300K equilibration and 80K recooling steps. Comparison of the IINS spectra with electron energy loss results on Pt(111) suggest that the 128 meV peak is indeed due to the Pt-O-H bending mode of adsorbed OH species present as the dominant hy-drogenous species on the Pt black surface for O:H ratios of unity.

100,433

PB91-237651 Not available NTIS National Inst. of Standards and Technology (CSTL), Boulder, CO. Thermophysics Div.

Extended Phase Rule for Nonreactive, Multiphase, Multicomponent Chemical Systems.

Final rept L. J. Van Poolen, 1990, 13p

Pub. in Fluid Phase Equilibria 58, n1-2 p133-145, 1 Jun

Keywords: \*Phase rule, \*Mixtures, Phase diagrams, Phase transformations, Degrees of freedom, Thermodynamics, Reprints, Total density, Total composition, Phase volume fractions.

A comprehensive phase rule for nonreacting, multicomponent, multiphase systems is developed which considers the system intensive variables, overall or total density, overall composition and phase volume fractions. This extended phase rule, especially as it incorporates overall density and composition, may be of use to engineers who design chemical processing equipment and to theoreticians concerned with the nature of thermodynamic equilibrium. The degrees of freedom are given as (C + 1) where (C) is the number of components. The Gibbs phase rule is incorporated into this formulation. For a single phase the system intensive variables are the same as phase intensive variables and the rule given here and that of Gibbs are coincident. When the maximum possible number of phase is present, e.g., for a pure substance at its triple point, only system intensive variables such as total density or phase volume fractions can be specified. For cases other than the single phase or maximum number of possible phases it is shown that no phase intensive variables need be specified to fix the state of thermodynamic equilibrium. However, in the case of vapor-liquid equilibria it is useful to fix the phase intensive variable temperature along with the system intensive variables total density and composition. Along such thermodynamic paths mixtures are seen to behave similarly to pure fluids in that the mixture can be represented by pure-fluid-like vapor pressure and coexistence density curves.

100.434

PB91-237693 Not available NTIS National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Ceramics Div. Database and Retrieval System for the NBS Tables of Chemical Thermodynamic Properties.

Final rept.

P. Wang, and D. B. Neumann. 1989, 8p

Pub. in Jnl. of Chemical Information and Computer Sciences 29, n1 p31-38 1989.

Keywords: \*Thermodynamic properties, \*Chemical properties, \*Information systems, Data base management, Inorganic compounds, Organic compounds, Information retrieval, Reprints.

The organization and structure of a database for the 'NBS tables of chemical thermodynamic properties Selected values for inorganic and C1 and C2 organic substances in SI units' is explained. The use of a commercial database management system for the storage and retrieval system is discussed. The file constructs necessary to provide rapid retrieval by elemental composition in the type of database management system are shown. Both implementations on a mini-computer and on personal computers are discussed.

100,435

PB91-237701 Not available NTIS National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Ceramics Div.

Surface Oxidation Kinetics of Si3N4 - 4% Y2O3 Powders Studied by Bremsstrahlung-Excited Auger Spectroscopy.

Final rept.

P. S. Wang, S. M. Hsu, S. G. Malghan, and T. N. Wittberg. 1991, 4p

Pub. in Jnl. of Materials Science 26, p3249-3252 1991.

Keywords: \*Oxidation, \*Reaction kinetics, \*Silicon nitrides, \*Ceramics, \*Auger electron spectroscopy, Powders, Surface chemistry, Yttrium oxides, Bremsstrahlung, Time dependence, Silicon oxides, Activation energy, Solid-solid interfaces, Sintering, Reprints.

Samples of silicon nitride powder containing 4.0% Y2O3 in weight were heated in air at temperatures between 900 and 1000 C. The average SiO2 layer thickness on the Si3N4 powder particles, as a function of time at a particular temperature, was measured by Bremsstrahlung-excited Auger electron spectroscopy. Oxidation was found to follow a linear rate law with an activation energy of 56 + or - 1.5 kcal/mol. The yttri-um level measured by X-ray photoelectron spectroscopy was also found to decrease as a function of the oxide layer thickness. This suggests that there is a reaction between the Si3N4 and Y2O3 particles which results in the formation of an yttrium-rich phase at the interface between the surface SiO2 layer and the underlying Si3N4 particle.

100,436

PB91-237719 Not available NTIS National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Ceramics Div.

Oxidation Kinetics of Silicon Carbide Whiskers Studied by X-ray Photoelectron Spectroscopy. Final rept.

P. S. Wang, S. M. Hsu, and T. N. Wittberg. 1991, 4p Pub. in Jnl. of Materials Science 26, p1655-1658 1991.

Keywords: \*Oxidation, \*Reaction kinetics, \*Silicon carbides, \*Ceramics, Whiskers, Photoelectron spectroscopy, X ray analysis, Surface chemistry, Thickness, Silicon oxides, Equations, Calculation methods, Activation energy, Measurement, Reprints.

Silicon carbide whisker surfaces were characterized by X-ray photoelectron spectroscopy (XPS) to determine changes in the surface oxide film which occurred as a result of heating in air at temperatures from 600 to 800 C. Equations were derived for the calculation of surface oxide film thickness from the SiC to SiO2 2p intensity ratios. Oxidation was found to follow a linear rate law in the temperature range for the first 10 nm of oxide growth. An activation energy of 17.2 + or - 2.8 kcal/mol (72 + or - 12 kJ/mol) was measured.

100,437

PB91-237784 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Center for Chemical Physics.

# **Physical & Theoretical Chemistry**

Rovibrational Analysis of the nu7(1) Intermolecular Hydrogen Bond Bending Vibration in HCN-HF Using Far Infrared Fourier Transform Spectrosco-

py.
Final rept.
B. A. Wofford, W. J. Lafferty, W. B. Olsen, R. S.
Ram, A. Quinonez, and J. W. Bevan. 1988, 6p
Pub. in Chemical Physics Letters 152, n4-5 p299-304

Keywords: \*Hydrogen bonds, \*Hydrogen cyanide, \*Hydrogen fluoride, \*Molecular vibration, \*Vibrational spectra, Infrared spectroscopy, Molecular structure, Reprints, \*Hydrogen bonded complexes, Rotational

The nu7(1) fundamental of the hydrogen bonded complex, HCN-HF, has been observed in the gas phase in the far infrared using a cooled static long path gas cell. The frequency of this intermolecular vibration is 73.5835(6)/cm. Rotational constants have been determined.

100,438 PB91-237859 Not available NTIS National Inst. of Standards and Technology (IMSE),

Gaithersburg, MD. Polymers Div.
Evaluation of Liquid Junction Potentials and Determination of pH Values of Strong Acids at Moderate Ionic Strengths.

Final rept. Y. C. Wu, W. F. Koch, and D. Feng. 1989, 9p Pub. in Jnl. of Solution Chemistry 18, n7 p641-649 1989

Keywords: \*Electric potential, \*pH, Electrochemistry, Inorganic acids, Solutions, Ionic strength, Reprints, \*Junction potential, Strong acids.

A new method is proposed for the evaluation of the liquid junction potential and the single ion activity. Neither of these quantities can be determined independently. However, the ratio of the activity coefficients may be evaluated by following the method suggested by Frank, from which the liquid junction potential may be computed, so also the pH values at higher ionic strengths (<1 m). Experimental results are presented and uncertainty is discussed.

100,439 PB91-237867 Not available NTIS Not available NTS National Inst. of Standards and Technology (CSTL), Gaithersburg, MD. Biotechnology Div. Electrochemical Behavior of Ferrocene in Polyeth-

ylene Oxide-400. Final rept. W. T. Yap, E. A. Blubaugh, R. A. Durst, and C. K.

Chiang. 1989, 4p Pub. in Jnl. of the Electrochemical Society 136, n9 p2588-2591 1989.

Keywords: \*Polyethylene glycols, \*Solid electrolytes, \*Conductive polymers, \*Ferrocene, \*Electrochemistry, Photovoltaic cells, Battery charging, Solutes, Electron transfer, Volt-ampere characteristics, Chemical reactions, Diffusion, Reprints.

There have been many studies on and applications of polymer-based (polyethylene oxides) solid electro-lytes. These polymeric electrolytes are utilized in areas, such as, solid state batteries and photovoltaic cells. The high boiling point of these polymer electro-lytes makes them potentially useful as solvents for electrochemical reactions at elevated temperatures. Additionally, the study of the physical properties for dissolved analyte such as, diffusion, chemical reactivi-ties are of more fundamental but important, in nature. Presented in the work are studies involving the electroactivity of ferrocene in polyethylene glycol-400. Discussions are included involving the relative contributions of electron transfer rates and uncompensated resistance to the current potential curves obtained in the studies.

PB92-110113 Not available NTIS American Chemical Society, Washington, DC.
Journal of Physical and Chemical Reference Data,

Journal of Physical and Chemical Reference Data, Volume 20, Number 1, 1991.

Bimonthly rept.
D. R. Lide. c1991, 202p
See also PB92-110121 through PB92-110154, PB92-110162, PB92-110212, and PB91-192542. Errata sheet inserted. Prepared in cooperation with American Inst. of Physics, New York. Sponsored by National Inst. of Standards and Technology, Gaithersburg, MD.

Available from American Chemical Society, 115 16th St., NW, Washington, DC. 20036-9976.

Keywords: \*Physical properties, Spectrum analysis, Tables (Data), Copper ions, Atomic energy levels, Magnesium, Alkyl compounds, Alkoxy compounds, Wavelengths, Enthalpy, Liquid crystals, lonization, Molecular structure, Hydrides, Diatomic molecules, Transition temperature, \*Reference materials, Benzoic acid/(phenyl-ester), Grotrian diagrams.

Contents:

Intents:

Spectral Data and Grotrian Diagrams for Highly Ionized Copper, Cu X-Cu XXIX;

Wavelengths and Energy Level Classifications of Magnesium Spectra for All Stages of Ionization (Mg I thru XII);

Spectroscopy and Structure of the Alkali Hydride Diatomic Molecules and Their Ions;

Critical Evaluation of Liquid Crystal Transition

Temperatures I: 4,4'-Alkyl/alkylphenylbenzoates; Cumulative listing of Reprints and Supplements.

100,441 PB92-110121

(Order as PB92-110113)
Japan Atomic Energy Research Inst., Tokai.
Spectral Data and Grotrian Diagrams for Highly
Ionized Copper, Cu X-Cu XXIX.
T. Shirai, T. Nakagaki, Y. Nakai, J. Sugar, and K.
Ishii. c1991 810

Ishii. c1991, 81p

Prepared in cooperation with National Inst. of Standards and Technology, Gaithersburg, MD., Kyoto Univ. (Japan), and Hiroshima-Denki Inst. of Tech. (Japan). Included in Jnl. of Physical and Chemical Reference Data, v20 n1 p1-81 1991. Available from American Chemical Society, 1155 16th St., NW, Washington, DC 20036 2076. DC. 20036-9976.

Keywords: \*Spectrum analysis, \*Copper ions, Wavelengths, Tables(Data), Atomic energy levels, Graphs(Charts), Ionization, \*Reference materials, \*Grotrian diagrams.

Wavelengths, energy levels, level classifications, intensities, and transition probabilities for the copper spectra Cu X to Cu XXIX are compiled. The data are critically evaluated and the best results, in the authors' judgement are quoted. A short review of the work on each stage of ionization is included. Grotrian diagrams are also presented to provide graphical overviews. The literature has been surveyed to March 1990. (Copyright (c) 1991 by the U.S. Secretary of Commerce.)

100,442 PB92-110139

(Order as PB92-110113) National Inst. of Standards and Technology, Gaithers-

National Inst. of Standards and Technology, Galarico burg, MD.

Wavelengths and Energy Level Classifications of Magnesium Spectra for All Stages of Ionization (Mg I through Mg XII).

V. Kaufman, and W. C. Martin. c1991, 70p Included in Jnl. of Physical and Chemical Reference Data, v20 n1 p83-152 1991. Available from American Chemical Society, 1155 16th St., NW, Washington, DC 20036-9976. DC. 20036-9976.

Keywords: \*Wavelengths, \*Spectrum analysis, \*Atomic energy levels, \*Magnesium, Tables(Data), Listings, Ionization, Critical point, \*Reference materi-

Wavelengths and their classifications are compiled for the spectra of magnesium. Selections of data are based on the critical evaluations in the compilation of energy levels by Martin and Zalubas with some updat-ing from the more recent literature. All classifications have been verified with predictions made by differencing the energy levels. In addition to the spectra or-dered by ionization stage, two finding lists are includ-ed, one containing Mg I to Mg III and the other Mg IV to Mg XII. (Copyright (c) 1991 by the U.S. Secretary of Commerce.)

100,443 PB92-110147

(Order as PB92-110113)

lowa Univ., Iowa City.
Spectroscopy and Structure of the Alkali Hydride Diatomic Molecules and Their Ions.
W. C. Stwalley, W. T. Zemke, and S. C. Yang. c1991,

Prepared in cooperation with Wartburg Coll., Waverley, IA. Dept. of Chemistry, and Rhode Island Univ., Kingston. Dept. of Chemistry.

Included in Jnl. of Physical and Chemical Reference Data, v20 n1 p153-187 1991. Available from American Chemical Society, 1155 16th St., NW, Washington, DC. 20036-9976.

Keywords: Spectrum analysis, \*Molecular structure, \*Metal hydrides, \*Diatomic molecules, \*Ions, Sodium hydrides, Potassium hydrides, Cesium hydrides, Atomic energy levels, Rubidium hydrides, Alkali metals, Hydrides, Deuterium compounds, Laser spectroscopy, Excitation, \*Reference materials.

All significant experimental measurements and theoretical calculations of the spectroscopy and structure of the alkali hydrides NaH, KH, RbH and CsH, and the corresponding alkali deuterides, are identified and reviewed. Published molecular constant determinations from conventional and laser spectroscopy are evaluatfrom conventional and laser spectroscopy are evaluated; recommended spectroscopic constants for Chi(1)Sigma(+) and Alpha(1)Sigma(+) states are tabulated. RKR and hybarid potential energy curves are evaluated; recommended RKR curves for CHI(1)Sigma(+) and Alpha(1)Sigma(+) states are tabulated. Ground state dissociation energy (De) estimates are evaluated; recommended Chi(1)Sigma(+) and Alpha(1)Sigma(+) state De and D6 values are tabulated. Accurate electronic structure calculations (Hartree-Eock or heter) are listed and described brief. (Hartree Fock or better) are listed and described briefly; all excited electronic states considered are included. Experimental and theoretical radiative and dipole properties are noted and discussed. Calculations on the positive and negative ions of the four diatomic alkali hydrides are also listed and described briefly. (Copyraight (c) 1991 by the U.S. Secretary of Commerce.)

100.444 PB92-110154

(Order as PB92-110113)

Kent State Univ., OH. Critical Evaluation of Liquid Crystal Transition Temperatures I: 4,4'-Alkyl/alkoxyphenylbenzoates.

T. T. Blair, M. E. Neubert, M. Tsai, and C. Tsai. c1991, 16p Included in Jnl. of Physical and Chemical Reference

Data, v20 n1 p189-204 1991. Available from American Chemical Society, 1155 16th St., NW, Washington, DC. 20036-9976.

Keywords: \*Liquid crystals, \*Transition temperatures, \*Alkyl compounds, \*Alkoxy compounds, Melting points, Enthalpy, Phase transformations, Tables(Data), Graphs(Charts), Error analysis, Molecular structure, \*Benzoic acid/(phenyl-ester).

Transition temperataures for 366 straight chain 4,43 alkyl/alkoxyphenylbenzoates (through Nov. 1990) have been compiled and critically evaluated. Information was obtained wherever possible, with the exception of the patent literature, and examined for editorial coherency. Line graphs of the melting and clearing temperatures were plotted as a function of the chain length of either side, while holding constant the other side, and evaluated for consistency, particularly for the persistence of the odd-even alternation in the clearing curve. It became apparent that major breaks in the curve indicated errors in the data which, when correctcurve indicated errors in the data which, when correct-ed, restored the alternating curve. Mesophase identification was reviewed by evaluating bar graphs and block diagrams. Usually, a given phase appeared first in a monotropic form, then in an enantiotropic form, and finally disappeared without reappearing in the series. Further evaluation of the data suggested that a number of phases have been missed. Evaluated transition temperatures are available on 38 dialkyl, 91 alkyl/alkoxy, 100 alkoxy/alkyl, and 137 dialkoxy compounds. Enthalpies for 93 of the esters are also included. (Copyright (c) 1991 by the U.S. Secretary of Commerce.) merce.)

100,445 PB92-110162 Not available NTIS American Chemical Society, Washington, DC.

Journal of Physical and Chemical Reference Data, Volume 20, Number 2, March-April 1991.

D. R. Lide. c1991, 234p See also PB92-110170 through PB92-110204, PB92-110212, PB92-110113, and PB91-192542. Prepared in cooperation with American Inst. of Physics, New York. Sponsored by National Inst. of Standards and Technology. nology, Gaithersburg, MD. Available from American Chemical Society, 1155 16th St., NW, Washington, DC. 20036-9976.

Keywords: \*Physical chemistry, Thermochemistry, Combustion, Propenes, Thermodynamic properties, Thermophysical properties, Ethane, Information systems, Specific heat, Polymers, Organic compounds, Liquid phases, Alkanes, \*Reference materials, ATHAS system.

Contents:

Chemical Kinetic Data Base for Combustion Chemistry Part V. Propene; Thermophysical Properties of Ethane;
Heat Capacity and Other Thermodynamic
Properties of Linear Macromolecules. X.
Update of the ATHAS 1980 Data Bank; Heat Capacities of Organic Compounds in Liquid State. II. C1 to C18 n-Alkanes; Cumulative Listing of Reprints and Supplements.

PB92-110170

(Order as PB92-110162) National Inst. of Standards and Technology (NML), Gaithersburg MD. Chemical Kinetics Div. Chemical Kinetic Data Base for Combustion Chem-

W. Tsang. c1991, 53p
Included in Jnl. of Physical and Chemical Reference
Data, v20 n2 p221-273 Mar/Apr 91. Available from
American Chemical Society, 1155 16th St., NW, Washington, DC. 20036-9976.

Keywords: \*Reaction kinetics, \*Combustion, \*Propenes, \*Thermochemistry, Inorganic compounds, Pyrolysis, Alkanes, Transport properties, Thermodynamic properties, Vapor phases, Tables(Data), \*Reference

The publication contains evaluated and estimated data on the kinetics of reactions involving propene and allyl radical and various small inorganic and organic species which are of importance for the proper under-standing of the early stages of propene and the inter-mediate stages of propane and isobutane combustion and pyrolysis. It is meant to be used on conjunction with the kinetic data given in earlier publications, which is of direct pertinence to the understanding of methane, ethane, methanol, propane and isobutane pyrolysis and combustion, but which also contains a large volume of data that are applicable to the propene system. The temperature range covered is 300-2500 K and the density range 10 to the 16th power to 10 to the 21st power molecules/cu cm. (Copyright (c) 1991 by the U.S. Secretary of Commerce.)

100.447 PB92-110188

(Order as PB92-110162) National Inst. of Standards and Technology (NML), Boulder, CO. Thermophysics Div. Thermophysical Properties of Ethane.

D. G. Friend, H. Ingham, and J. F. Ely. c1991, 73p Included in Jnl. of Physical and Chemical Reference Data, v20 n2 p275-347 Mar/Apr 91. Available from American Chemical Society, 1155 16th St., NW, Washington, DC. 20036-9976.

Keywords: \*Thermophysical properties, \*Ethane, Liquid phases, Thermodynamic properties, Equations of state, Transpoort properties, Specific heat, Tables(Data), Boundary layer transition, Phase rule, Viscosity, Ideal gas, Thermal conductivity, \*Reference materials.

New correlations for the thermophysical properties of fluid ethane are presented. The correlations are based on a critical evaluation of the available experimental data and have been developed to represent these data over a broad range of the state variables. Estimates for the accuracy of the equations and comparisons with measured properties are given. The reasons for the new study of ethane include significant new and accurate data and improvements in the correlating functions which allow increased accuracy of the correlations--especially in the extended critical region. Short tables of the thermophysical properties of ethane are included. The study complements an earlier study of methane and uses the same correlating equations and format. (Copyright (c) 1991 by the U.S. Secretary of Commerce.)

100,448 PB92-110204

(Order as PB92-110162) Vysoka Skola Chemicko-Technologicka, Prague (Czechoslovakia). Heat Capacities of Organic Compounds in Liquid State. 2. C1 to C18 n-Alkanes. V. Rizicka, M. Zabransky, and V. Majer. c1991, 52p

Prepared in cooperation with Clermont-Ferrand-2 Univ., Aubiere (France).

Included in Jnl. of Physical and Chemical Reference Data, v20 n2 p405-444 Mar/Apr 91. Available from American Chemical Society, 1155 16th St., NW, Washington, DC. 20036-9976.

Keywords: \*Specific heat, \*Organic compounds, \*Al-kanes, \*Liquid phases, Thermodynamic properties, Tables(Data), Experimental design, Least square methods, Temperature, \*Reference materials.

Heat capacities of liquid C1 to C18 n-alkanes measured by calorimetric methods have been compiled and evaluated. The selected experimental data were fitted as a function if temperature with cubic splines using weighted least squares minimization. The parameters of the cubic spline polynomials and the recommended values for heat capacities are presented. Heat capacities were also fitted by a quasipolynomial equation permitting extrapolation of heat capacities outside the temperature range of experimental values. (Copyright (c) 1991 by the U.S. Secretary of Commerce.)

PB92-110212 Not available NTIS American Chemical Society, Washington, DC.
Journal of Physical and Chemical Reference Data, Volume 20, Number 3, May-June 1991.

Bimonthly rept.
D. R. Lide. c1991, 128p
See also PB92-110220 through PB92-110253, PB92-110113 and PB92-110162. Prepared in cooperation with American Inst. of Physics, New York. Sponsored by National Inst. of Standards and Technology, Gaithersburg, MD.

Available from American Chemical Society, 1155 16th St., NW, Washington, DC 20036-9976.

Keywords: \*Physical chemistry, Argon ions, Nitrogen, Reaction kinetics, Vapor phases, Thermodynamic properties, Nitroxyl radicals, Organic compounds, Sodium bromides, Argon, Nitrogen ions, Atomic energy levels, Ion-molecule collisions, Molecule-molecule collisions, Solubility, Carbon dioxide, Critical point, Water, Cross sections, \*Reference materials, Chemical reaction mechanisms.

Kinetics and Mechanisms of the Gas-Phase Reactions of the NO3 Radical with Organic Compounds;

Thermodynamic Properties of the NaBr+H2O System:

Cross Sections and Swarm Coefficients for Nitrogen Ions and Neutrals in N2 and Argon lons and Neutrals in Ar for Energies from 0.1 eV to 10 keV:

Evaluation of Solubility Data of the System CO2-H2O from 273 K to the Critical Point of Water; Cumulative Listing of Reprints and Supplements.

100,450 PB92-110220

(Order as PB92-110212) California Univ., Riverside. Statewide Air Pollution Research Center.

Kinetics and Mechanisms of the Gas-Phase Reac-

tions of the NO3 Radical with Organic Compounds.

R. Atkinson. c1991, 49p Included in Jnl. of Physical and Chemical Reference Data, v20 n3 p459-507 May/Jun 91. Available from American Chemical Society, 1155 16th St., NW, Washington, DC 20036-9976.

Keywords: \*Reaction kinetics, \*Nitroxyl radicals, \*Organic compounds, Vapor phases, Reviews, Chemical reactions, Free radicals, Nitrates, \*Chemical reaction mechanisms, \*Reference materials.

A substantial data base concerning the rate constants for the gas-phase reactions of the nitrate (NO3) radical with organic compounds is now available, with rate constants having been determined using both absolute and relative rate methods. To date, the majority of these kinetic data have been obtained at room temperature using relative rate techniques utilizing both the reactions of the NO3 radical with other organic compounds and the equilibrium constants for the NO3+NO2 in equilibrium with N205 reactions as the reference reaction. In the article, the literature kinetic and mechanistic data for the gas-phase reactions of the NO3 radical with organic compounds (through late

1990) have been tabulated, reviewed and evaluated. While the available data base exhibits generally good agreement and self-consistency, further absolute rate data are needed, preferably as a function of tempera-ture. Most importantly, mechanistic and product data for the reactions of the NO3 radical with organic compounds need to be obtained. (Copyright (c) 1991 by the U.S. Secretary of Commerce.)

100.451

PB92-110238

(Order as PB92-110212) National Inst. of Standards and Technology, Gaithers-

Thermodynamic Properties of the NaBr + H2O System.

D. G. Archer. c1991, 47p

Data, v20 n3 p509-555 May/Jun 91. Available from American Chemical Society, 1155 16th St., NW, Washington, DC 20036-9976.

Keywords: \*Thermodynamic properties, \*Sodium bromides, \*Water, Chemical reactions, Experimental design, Thermodynamic activity, Reaction kinetics, Gibbs free energy, Enthalpy, Entropy, \*Reference ma-

Equations that described the thermodynamic properties of the NaBr + H2O system were obtained from a fit to experimental results for the system. The experimental results included in the fit spanned the range of temperature of approximately 260 to 623 K and the range of pressure from the vapor pressure of the solu-tion to 150 MPa. New equations and/or values for the following properties are given in the present work: (1) the change in chemical potential with respect to temperature and pressure for NaBr(cr), valid from 200 to 900 K. (2) delta(sub f)G(sub m) and delta(sub f)H(sub m) from the elements, as well as S(sub m) and C(sub p, m), all for 298.15 K, 0.1 MPa for NaBr:2H2O(cr), (4) the change in chemical potential for both NaBr and H2O in NaBr(aq) as a function of temperature, pressure, and molality, valid from 260 to 600 K and from the vapor pressure of the solution to 150 MPa. (Copy-right (c) 1991 by the U.S. Secretary of Commerce.)

100,452 PB92-110246

(Order as PB92-110212)

(Order as PB92-110212) Joint Inst. for Lab. Astrophysics, Boulder, CO. Cross Sections and Swarm Coefficients for Nitrogen Ions and Neutrals in N2 and Argon Ions and Neutrals in N2 and Argon Ions and Neutrals in Ar for Energles from 0.1 eV 10 keV.

A. V. Phelps. c1991, 17p
Included in Jnl. of Physical and Chemical Reference Data, v20 n3 p557-573 May/Jun 91. Available from American Chemical Society, 1155 16th St., NW, Washington, DC 20036-9976.

ington, DC 20036-9976.

Keywords: \*Ion-molecule collisions, \*Molecule-molecule collisions, \*Cross sections, Nitrogen ions, Nitrogen, Argon ions, Argon, Atomic energy levels, Charged-particle transfer, Reaction kinetics, Excition, Tables(Data), Graphs(Charts).

Graphical and tabulated data and the associated bibliography are presented for cross sections for elastic, excitation, and ionization collisions of N(+), N2(+), N, and N2 with N2 and for Ar(+) and Ar with Ar for laboratory energies from 0.1 eV to 10 keV. Where appropriate, drift velocities and reaction or excitation coefficients are calculated from the cross sections and recommended for use in analyses of swarm experiments and electrical discharges. In the case of N(+) in N2, cross sections for momentum transfer, charge transfer, electronic excitation, and electron production are recommended. In the case of N in N2, only cross sections for momentum transfer are recommended. For N2 in N2, cross sections for momentum transfer, electronic excitation, and electron production are recommended. Collisions of electronically excited states with N2 are not included. For Ar(+) in Ar, cross sections for charge transfer, electronic excitation, and electron production are recommended. For Ar in Ar, cross sections for momentum transfer, electronic excitation, and electron production are recommended.

100 453 PB92-110253

(Order as PB92-110212) National Inst. of Standards and Technology (NML), Gaithersburg, MD. Thermophysics Div.

# **Physical & Theoretical Chemistry**

Evaluation of Solubility Data of the System CO-H2O from 273 K to the Critical Point of Water.

R. Crovetto. c1991, 15p
Included in Jnl. of Physical and Chemical Reference
Data, v20 n3 p575-589 May/Jun 91. Available from
American Chemical Society, 1155 16th St., NW, Washington DC 20036-9276 ington, DC 20036-9976.

Keywords: \*Solubility, \*Carbon dioxide, \*Water, High temperature tests, Critical point, Pressure, Henry's law, Equations of state, Vapor phases.

The critical review covers the existing literature on the solubility of CO2 in water from 273 K to the critical temperature of the solvent (647 K). Results of the evaluation are expressed in the form of fitting equations for the infinite dilution Henry's constant, k, as a function of the density of the solvent, and also as an explicit func-tion of the temperature. The pressure effect on the solubility is considered in the formulation. Different equations of state were used for the description of the CO2-H2O vapor phase and the effect on the calculated Henry's constant values are analyzed. The 'best' solu-bility estimates are presented in smoothed tabular form. (Copyright (c) 1991 by the U.S. Secretary of Commerce.)

100,454 PB92-116326 PC A03/MF A01
National Inst. of Standards and Technology (CSTL),
Boulder, CO. Chemical Engineering Div.
Transient Hydrogen Heat Transfer. Final Report
for April 1986-April 1989.
B. Louie, and W. G. Steward. Oct 91, 42p NISTIR-

Contract WPAFB MIPR FY1455-89-N0604 See also PB90-254764. Prepared in cooperation with FluidTherm Engineering, Boulder, CO.

Keywords: \*Liquid hydrogen, \*Heat transfer, Cryogenics, Transients, Thin films, Carbon, Platinum, Heat of vaporization, Nucleate boiling, Heat measurement, Substrates, Ceramics, Aluminum oxide, Quartz, Glass expoxy composites, Electric conductivity, Power gen-

Transient heat transfer to liquid hydrogen was investigated. Thin carbon films and Pt foils submerged in liquid hydrogen received stepped inputs of power ranging from 1 to 42 W/sq cm, and the onset of nucleate or film boiling was obtained for each power level. The critical heat flux was found to be approximately 8 W/sq cm, with the transition to film boiling occurring in W/sq cm, with the transition to film boiling occurring in times less than 0.00 s. Premature film boiling can be related to the positive temperature coefficient of resistance and the narrowness of the heaters. Thermometric devices and power generation equipment selection are discussed.

100,455 PB92-116508 Not available NTIS National Inst. of Standards and Technology (NML),

Boulder, CO. Thermophysics Div.

Hydrogen Component Fugacity Coefficients in Binary Mixtures with Etane: Pressure Dependence. Final rept.

T. J. Bruno, J. A. Schroeder, and S. L. Outcalt. 1990, See also PB89-124853. Sponsored by Gas Research

Inst., Chicago, IL.
Pub. in International Jnl. of Thermophysics 11, n5 p889-896 1990.

Keywords: \*Fugacity, \*Binary mixtures, \*Hydrogen, \*Ethane, Test chambers, Comparison, Reprints.

The fugacity coefficients of hydrogen in binary mixtures with ethane were measured. Data were taken using an experimental chamber which is divided into two regions by a semipermeable membrane through which hydrogen, but not ethane can penetrate. The measurement of the gas pressures inside and outside the membrane gives the hydrogen component fugacity at a given temperature, binary mixture mole fraction, and mixture pressure. In the paper, results are reported at mixture pressures of 5.25, 6.97, 10.21, and 13.47 MPa. In each case, the temperature of the mixture was maintained at an average value of 130 C (403.15K). The general qualitative features of the data are discussed, and comparisons are made with predictions obtained from the Redlich-Kwong and Peng-Robinson equations of state.

PB92-116524 Not available NTIS National Inst. of Standards and Technology (CSTL), Boulder, CO. Chemical Engineering Div.

Thermodynamics of the Divalent-Metal Fluorides. 4. Heat Capacity of MSnF4, M=Pb, Ba, or Sr, at Temperatures from 300 K to 660 K.

Final rept. J. E. Callanan, and R. D. Weir. 1991, 10p See also PB91-149864. Sponsored by Department of National Defence, Ottawa (Ontario).
Pub. in Jnl. of Chemical Thermodynamics 23, p411-

Keywords: \*lonic conductivity, \*Calorimetry, \*Specific heat, \*Stannates, Thermodynamic properties, Temperature dependence, Strontium compounds, Barium compounds, Lead compounds, Phase transformations, Monoclinic lattices, Tetragonal lattices, Cubic lattices, Fluorine 19, Enthalpy, Entropy, Transition temperature, Reprints, \*Fast ion conductors, Tetrafluorostannates.

The low-temperature adiabatic calorimetric measure-ments on three fast-ion conductors have been extended to 660 K by differential scanning calorimetry (d.s.c.). For strontium tetrafluorostannate SrSnF4 the heat capacities from the d.s.c. merged smoothly with those from the adiabatic measurements and no phase transition was observed up to 660 K. The anomaly between 280 K and 350 K was confirmed and a second anomaly was found near 475 K coincident with changes in the spin-lattice relaxation time of (19)F. The heat capacity of BaSnF4 rose smoothly from the anomaly between 210 K and 320 K noted previously in the adiabatic measurements. No evidence of a phase transition was observed up to 660 K, although the slope of the heat capacity against temperature curve increased above 510 K. In lead tetrafluorostannate PbSnF4 the transition from the monoclinic alpha-PbSnF4 the transition from the monoclinic alpha-phase to tetragonal beta-phase was complete at 365 K with an associated enthalpy = (306.0 + or - 0.2) J/ mol and entropy = (0.97 + or - 0.02) J/K/mol. The heat capacity then rose smoothly to 500 K where it increased sharply leading up to the tetragonal beta-phase to cubic gamma-phase transition at 600 K with enthalpy = (2.53 + or - 0.02) kJ/mol and entropy = (4.03 + or - 0.05) J/K/mol. Thermodynamic functions are tabulated to 600 K for SrSnF4 and to 650 K for RaSnF4 and PbSnF4 BaSnF4 and PbSnF4.

100,457 PB92-116649 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Molecular Physics Div.
Rotational-Tunneling Spectrum of the Ar-SO2 van der Waals Complex. Final rept.

L. H. Coudert, K. Matsumura, and F. J. Lovas. 1991, Pub. in Jnl. of Molecular Spectroscopy 147, p46-60

Keywords: \*Microwave spectra, \*Argon compounds, \*Sulfur dioxide, Gases, Molecular structure, Spectrum analysis, Fourier transformation, Fabry-perot interferometer, Sulfur 32 reactions, Sulfur 34 reactions, Rotational states, Coriolis force, Reprints.

The microwave spectrum of Ar-So2 has been observed with a pulsed beam, Fabry-Perot cavity, Fourier transform microwave spectrometer. This complex dis-plays a- and c-type spectra, the latter of which is shifted by internal motion of the SO2 unit. In addition to the ed by internal motion of the SO2 unit. In addition to the spectrum of the normal isotopic form, the spectrum of Ar- (34) SO2 was observed. Rotational analysis of each spectrum provides the constants A = 9151.235(5) MHz, 1/2 (B + C) = 1402.0444 (3) MHz, and B - C = 167.808 (2) MHz for the normal species, and A = 9112.734 (6) MHz, 1/2 (B + C) = 1385.149 (6) MHz, and B - C = 162.838 (2) MHz for the Ar - (34) SO2 species. Constants relevant to the Coriolis coupling between the tunneling motion and the overall rotation of the molecule are also determined and, along with the rotational constants, make possible an unamwith the rotational constants, make possible an unambiguous determination of the angle between the a axis of the complex and the C2 axis of the SO2 molecule.

PB92-116839 Not available NTIS
National Inst. of Standards and Technology (NML),
Gaithersburg, MD. Thermophysics Div.
Apparatus for Acoustic Measurements of Gases
with Applications of High Temperatures with Applications for High Temperatures. Final rept.

Final rept.
K. A. Gillis, and M. R. Moldover. 1991, 8p
Contracts DE-Al05-88ER13823, N0002490MP33493
Sponsored by Department of Energy, Washington, DC., and Department of the Navy, Washington, DC.

Pub. in Proceedings of Symposium on Energy Engineering Sciences Fluid and Dynamical Systems (9th), Argonne, IL., May 13-15, 1991, p310-317.

Keywords: \*Sound waves, \*Gases, \*Sound transducers, Specific heat, Virial equation, Thermodynamic properties, High temperature tests, Refrigerants, Reprints, Bid(diffuoromethyl) ether.

Accurate measurements of the speed of sound in gases are conventionally made using metal resonators with small transducers embedded in their walls. The authors have extended the method to include gases at high temperatures and gases that are corrosive or incompatible with elastomers and thermoplastics. The authors use remote transducers coupled to a resonaadultions desirable translated sources coupled to a resoluta-tor through acoustic waveguides. Thin metal dia-phragms separate the waveguides from the resonator and confine the test gas within an all-metal environ-ment. In the present apparatus, any gas compatible with gold and stainless steel can be studied. The apparatus was tested by determining the ideal-gas heat capacity and second acoustic virial coefficient of bis(difluoromethyl) ether. The ether is an environmentally benign compound; however, its solubility in polymer o-rings made it incompatible with conventional acoustic apparatus containing elastomers.

PB92-116854 Not available NTIS

Not available NTIS
National Inst. of Standards and Technology (CSTL),
Gaithersburg, MD. Biotechnology Div.
Thermodynamics of the Disproportionation of
Adenosine 5'-diphosphate to Adenosine 5'-triphosphate and Adenosine 5'-monophosphate. 1. Equilibrium Model.

Final rept. R. N. Goldberg, and Y. B. Tewari. 1991, 21p Pub. in Biophysical Chemistry 40, p241-261 1991.

Keywords: \*Disproportionation, \*Enzymes, \*Adenosine phosphates, \*ADP, \*Magnesium ions, \*ATP, Activity coefficients, Thermodynamic equilibrium, Mathematical models, Specific heat, AMP, Enthalpy, Blood cells, Nucleotides, Protons, Gibbs free energy, Hemoglobin, Catalysts, Biochemistry, Entropy, Reprints, Adenylate kinase, Ionic strength.

The thermodynamic treatment of the disproportionation reaction of adenosine 5 diphosphate to adeno-sine 5 triphosphate and adenosine 5 monophos-phate is discussed in terms of an equilibrium model which includes the effects of the multiplicity of ionic and metal bound species and the presence of long range electrostatic and short range repulsive interac-tions. Calculated quantities include equilibrium constants, enthalpies, heat capacities, entropies, and the stoichiometry of the overall reaction. The matter of how these calculations can be made self-consistent with respect to both calculated values of the ionic strength and the motality of the free magnesium ion is discussed. The thermodynamic data involving proton and magnesium-ion binding data for the nucleotides involved in this reaction have been evaluated.

100,460 PB92-117035 PB92-117035 Not available NTIS National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Ceramics Div.

Surface X-ray Absorption Spectroscopy, EXAFS and NEXAFS, for the In situ and Ex situ Study of Electrodes.

Final rept.

Final rept.
G. G. Long, and J. Kruger. 1991, 43p
Sponsored by National Science Foundation, Washington, DC., and Air Force Office of Scientific Research, Bolling AFB, DC.
Bub is Techniques for Characterization of Floritodes.

Pub. in Techniques for Characterization of Electrodes and Electrochemical Processes, Chapter 4, p167-209

Keywords: \*Electrodes, \*Surface chemistry, \*Electrochemistry, Corrosion inhibitors, X ray analysis, Reviews, On-line measurement systems, Characterization, Passivity, Electrolytes, Reprints, Extended x-ray absorption fine structure.

The report is a review of extended x-ray absorption fine structure (EXAFS) and NEXAFS spectroscopy as it applies to important issues in electrochemistry. The theory and the resolution of some of the problems encountered are given. Techniques and instrumentation are reviewed. And finally, examples are given of applications from passivity, corrosion inhibitors and batter-

100,461 PB92-117050 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Thermophysics Div. Semiclassical Calculation of Self-Broadening in O2, N2, and CO Raman Spectra.

Final rept.

J. P. Looney, and G. J. Rosasco. 1991, 12p Sponsored by Army Research Office, Research Trian-

gle Park, NC. Pub. in Jnl. of Chemical Physics 95, n4 p2379-2390, 15

Keywords: \*Raman spectra, \*Oxygen, \*Nitrogen, \*Carbon monoxide, Semiclassical approximation, Calculation methods, Spectrum analysis, Temperature dependence, Gases, Line broadening, Reprints.

Semiclassical calculations of the J and temperature dependence of the Raman Q1 and S0 self-broadened linewidths of O2, N2, and CO have been performed within the framework of Robert and Bonamy with J=0-30 and T=300-1500 K. The calculation of the CO self-broadened R1 linewidths are also reported for T = 100-300 K and J = 0-20. Comparison of the results of these calculations with recent experiments shows good overall agreement.

100.462 PB92-117092 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Semiconductor Electronics Div.

XANES of Transition Metal Zinc-Blende Semiconductors. Final rept.

D. A. McKeown. 1991, 3p Pub. in X-ray Absorption Fine Structure, Chapter 85, p346-348 1991.

Keywords: \*X ray analysis, \*Electron transitions, Semiconductors(Materials), \*Transition metals, Sulfides, Iron compounds, Copper compounds, Zinc compounds, Chalcopyrite, Sphalerite, Atomic structure, Reprints, X ray absorption near-edge structure, Zinc blende

XANES (X-ray absorption near-edge structure) is known to be sensitive to both the arrangement of atoms around, as well as the atomic states of the ab-sorbing atom. Therefore, it is not surprising that XANES data, collected on compounds having different arrangements of atoms around the absorbing atom, can have very different features. In the study, XANES data were gathered for three transition metals: Fe and Cu in chalcopyrite (CuFeS2), and Zn in sphalerite (ZnS), where all three cations are in nearly identical atomic environments (similar to the zinc-blende type structures in III-V semiconductors). Since the environments are similar, any change in the XANES should, to first approximation, be due entirely to atomic effects of the absorbing atom. The rationale behind the study is to see if any changes in the near-edge data can be assigned to electronic transitions of the absorbing atom; this may be useful for interpreting XANES for IIIv semiconductors. Previously, Zn, Cu, and Fe edges were presented separately, but no comparisons or calculations have been made for all three edges.

100,463 PB92-117175 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Molecular Physics Div. High-Resolution Infrared Spectrum of the nu1 Band of OC1O. Final rept.

Howard, and W. J. Lafferty. 1991, 25p Pub. in Jnl. of Molecular Spectroscopy 148, p346-370

Keywords: \*Chlorine oxides, \*Infrared spectra, High resolution, Absorption spectra, Band spectra, Reprints, Fourier transform infrared spectroscopy.

The infrared absorption spectrum of the nu(sub 1) band of OCIO (care must be taken to distinguish it from CIOO, which also exists) has been recorded in the 950/cm region, with a Fourier transform infrared spectrometer with an instrumental resolution of about 0.004/cm. Most lines appear as doublets owing to the spin-rotation interaction present in this molecule. Around 2800 lines have been assigned for the (35)CIO2 species and about 800 for the (37)CIO2 species. In addition, a number of lines of the 'hot band' nu(sub 1) + nu(sub 2) - nu(sub 2) have been assigned

for the (35)CIO2 species. Effective rotational and spinrotational spectroscopic constants have been obtained for the ground and the nu(sub 1) - 1 vibrational states of (35) ClO2 and (37)ClO2 and the corresponding band origins have also been determined. Fermi resonance between the 2nu(sub 2) and nu(sub 1) bands has been found to be negligible; however, a weak resonance between the K(sub alpha) = 7 levels of  $nu(sub\ 1) = 1$  and the K(sub alpha) = 9 levels of  $nu(sub\ 2) = 2$  has been observed. The measured integrated nu(sub 1) band strength is 87 + or - 6/sq cm/ atm at 300 K.

100.464 PB92-117290 Not available NTIS National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Metallurgy Div.

Laser Vaporization Mass Spectrometry of Refractory Materials: Graphite and YBa2Cu3Ox. Final rept.

P. K. Schenck, D. W. Bonnell, and J. W. Hastie.

1989, 5p Pub. in Jnl. of Vacuum Science and Technology A 7, n3 p1745-1749 1989.

Keywords: \*Graphite, Laser target interactions, High temperature superconductors, Mass spectroscopy, Reaction kinetics, Thermochemistry, Vaporization, Targets, Plumes, Reprints, \*Yttrium barium cuprates.

A very high pressure sampling mass spectrometer has been used to study the thermochemistry and kinetics of laser induced plumes from graphite and YBa2Cu3O(x) targets. Time resolved mass spectra of C(sub n) (n=1-9) neutral vapor species were obtained from graphite targets under conditions of varying laserfrom graphite targets under conditions of varying laser-surface interaction geometry and vapor plume-sam-pling geometry. Ionic species C1(1+), C2(1+), C3(1+), and impurities Na(1+) and K(1+) were also observed in the laser induced plume. Mass spectra obtained from superconducting YBa2Cu3O(x) targets showed an abundance of species in the laser induced plumes including both neutral and ionic Y, Ba, and Cu. In addition, species such as BaO, CuO(1+), YO and bimetallics (BaCu, YCu) were observed. Similar neutral and ionic metal atom species were observed using time resolved optical spectroscopy of the plume.

100.465 PB92-123157 PC A04/MF A01 National Inst. of Standards and Technology, Gaithersburg, MD. NIST X-Ray Photoelectron Spectroscopy (XPS)

Database. Technical note (Final).

C. D. Wagner. Oct 91, 62p NIST/TN-1289 Also available from Supt. of Docs. as SN003-003-03104-6. Prepared in cooperation with Surfex Co., Oakland, CA.

Keywords: \*X ray photoelectron spectroscopy, \*Photoelectron spectroscopy, \*Data bases, \*Bibliogratoelectron spectroscopy, \*Data bases, \*Bibliographies, Chemical shift, Binding energy, Auger electrons, Tables(Data).

The technique known as XPS (X-Ray Photoelectron Spectroscopy) involves x-ray irradiation of surface samples under high vacuum. Electrons escaping from the samples are sorted and arranged to form a spec-trum. A compilation of data for binding energy and ki-netic energy of sample electrons from all elements has been collected. Depending on the nature of the chemical bond, the chemical shift can be as much as 10 eV. Over the past 6 years the author has indexed articles related to the subject area. The data bank contains a total of 13,200 records, from a total of 800 papers.

100,466 PB92-148063 Not available NTIS American Chemical Society, Washington, DC.

Journal of Physical and Chemical Reference Data, Volume 20, Number 4, July/August 1991. Bimonthly rept.

Bimonthly rept.

D. R.: Lide. c1991, 168p
See also PB92-148071 through PB92-148105 and PB92-110212. Prepared in cooperation with American Inst. of Physics, New York. Sponsored by National Inst. of Standards and Technology, Gaithersburg, MD. Available from American Chemical Society, 115 16th St., NW, Washington, DC. 20036-9976.

Keywords: \*Physical chemistry, Supercritical fluids, Reaction kinetics, Combustion, Propellants, Molecular orbitals, Thermodynamic properties, Cyclopentadiene, Solutes, Liquids, Solids, Solubility, Nitrogen, Oxygen,

Molecular vibration, Molecular rotation, Constants, Carbon dioxide, Ab-initio calculations.

Contents:

Chemical Kinetic Data Base for Propellant Combustion. I. Reactions Involving NO, NO2, HNO, HNO2, HCN, and N2O;

Ab-Initio Calculations and Ideal Gas Thermodynamic Functions of Cyclopentadiene and Cyclopentadiene Derivatives;

Improved Fits for the Vibrational and Rotational Constants of Many States of Nitrogen and Oxygen;

Solubilities of Solids and Liquids of Low Volatility in Supercritical Carbon Dioxide.

100.467

PB92-148071

(Order as PB92-148063) National Inst. of Standards and Technology (NML), Gaithersburg, MD. Chemical Kinetics Div. Chemical Kinetic Data Base for Propellant, Com-

bustion. 1. Reactions Involving NO, NO2, HNO, HNO2, HCN and N2O.

W. Tsang, and J. T. Herron. c1991, 55p Included in Jnl. of Physical and Chemical Reference Data, v20 n4 p609-663 Jul/Aug 91. Available from American Chemical Society, 1155 16th St., NW, Washington, DC, 20036-9976.

Keywords: \*Reaction Kinetics, \*Combustion, \*Propellants, Transport properties, Nitrogen oxides, Chemical equilibrium, Chemical reactions, Hydrogen, Oxygen, Oxygen compounds, Carbon monoxide, RDX, Explosives, Cyanides, Tables(Data).

The publication contains evaluated chemical kinetic data on a number of single elementary reactions in-volving small polyatomic molecules which are of importance in propellant combustion. The work involves the collection and evaluation of mechanistic and rate information and the use of various methods for the extrapolation and estimation of rate data where information does not exits. The conditions covered range from tion does not exist. Ine conditions covered range from 500-2500K and 10 to the 17 power - 10 to the 22 power particles/cu cm. The results of the first years effort lead to coverage of all pertinent reactions of the following species; H, H2, H2O, O, OH, HCHO, CHO, CO, NO, NO2, HNO HNO2, HCN, and N2O. (Copyright (c) 1991 by the U.S. Secretary of Commerce.)

100.468

PB92-148089

(Order as PB92-148063) Technion - Israel Inst. of Tech., Haifa.

Ab-Initio Calculations and Ideal Gas Thermodynamic Functions of Cyclopentadiene and Cyclopentadiene Derivatives.

M. Karni, I. Oref, and A. Burcat. c1991, 19p Included in Jnl. of Physical and Chemical Reference Data, v20 n4 p665-683 Jul/Aug 91. Available from American Chemical Society, 1155 16th St., NW, Washington, DC. 20036-9976.

Keywords: \*Thermodynamic properties, \*Molecular orbitals, \*Cyclopentadiene, Cycloalkenes, Combustion, Fuels, Ideal gas, Molecular structure, Enthalpy, Thermochemistry, Entropy, Free radicals, Tables(Data), Moments of inertia, Molecular vibrations, Specific heat, \*Ab-initio calculations.

Analysis of recent experiments in combustion kinetics of cyclopentene (6), requires knowledge of the thermodynamic parameters of cyclopentadienyl radicals. Structures, frequencies and energies, ideal gas thermodynamic properties and values, have been calculated for cyclopentadiene, cyclopentadienols, and a number of radicals derived from them. The necessary molecular information for these calculations was found by ab-initio molecular orbital calculations. The geometries, vibrational frequencies and moments of inertia of 8 species are reported. In order to estimate the accuracy of the computations the molecular parameters were compared with known values reported in the literature whenever those were available. (Copyright (c) 1991 by the U.S. Secretary of Commerce.)

100.469

PB92-148097

(Order as PB92-148063)

R and D Associates, Los Angeles, CA.

# Physical & Theoretical Chemistry

Improved Fits for the Vibrational and Rotational Constants of Many States of Nitrogen and Oxygen. R. R. Laher, and F. R. Gilmore. c1991, 28p Contract DNA-001-88-C-0046

Sponsored by Defense Nuclear Agency, Washington,

Included in Jnl. of Physical and Chemical Reference Data, v20 n4 p685-712 Jul/Aug 91. Available from American Chemical Society, 1155 16th St., NW, Washington, DC. 20036-9976.

Keywords: \*Nitrogen, \*Oxygen, \*Molecular vibration, \*Molecular vibration, \*Molecular rotation, \*Constants, Molecular energy levels, Excitations, lons, Graphs(Charts), Tables(Data), Spectrum analysis.

All pertinent measurements of the vibrational intervals delta G (upsilon + 1/2) and rotational constants b(sub upsilon) for 11 states of N2, four states of N2(+), the ground state of O2, and four states of O2(+) that could be found in published papers have been assembled and plotted against upsilon. (These are the states important in modeling the fluorescence produced when air is bombarded by fast electrons.) These values of delta G and B(sub upsilon) are compared with values calculated from the standard polynomials in powers of upsilon + 1/2, using the coefficients tabulated by Huber and Herzberg (1979), as well as coefficients derived by later analysts, when available. In about 25 percent of the states considered, the coefficients of Huber and Herzberg are found to still yield good fits to the latest available spectroscopic data. In another 25 percent, good fits are obtained from more recently published coefficients. For the remaining 50 percent of the states, new improved coefficients have been derived by least-squares fitting. The results are tabulated and plotted. (Copyright (c) 1991 by the U.S. Secretary of Commerce.)

100,470 PB92-148105

(Order as PB92-148063)

Leeds Univ. (England).
Solubilities of Solids and Liquids of Low Volatility in Supercritical Carbon Dioxide.

K. D. Bartle, A. A. Clifford, S. A. Jafar, and G. F. Shilstone. c1991, 42p Included in Jnl. of Physical and Chemical Reference Data, v20 n4 p713-756 Jul/Aug 91. Available from American Chemical Society, 1155 16th St., NW, Washipton DC 2013-9276 ington, DC. 20036-9976.

Keywords: \*Carbon dioxide, \*Solubility, \*Solids, \*Liquids, \*Solutes, Supercritical fluids, Temperature, Pressure, Tables(Data), Gravimetric analysis, Chromato-graphic analysis, Phase studies, Phase stability, Equa-tions of state, Graphs(Charts), Spectrum analysis.

A table is given of the compounds of low volatility, whose experimental solubilities in supercritical carbon dioxide have been published up to the end of 1989, with the temperature and pressure ranges of the ex-perimental measurements, the experimental method, and references to the source of data. The data for pure compounds, which were presented in tabular form in the original publications, are shown in a series of fig-ures along with correlation lines for each isotherm. The method of correlation was to fit the experimental data for each isotherm, in the form of the natural logarithm of the product of mole fraction and pressure, to a linear function of density above a pressure of 100 bars. The constants obtained from the fitting procedures are given in a table. Procedures for estimating, from these constants, the solubilities of the compounds at temperatures and pressures different from those of the experimental data are suggested. (Copyright (c) 1991 by the U.S. Secretary of Commerce.)

PR92-148113 Not available NTIS American Chemical Society, Washington, DC.
Journal of Physical and Chemical Reference Data,

Volume 20, Number 5, September/October 1991.
Bimonthly rept.
D. R. Lide. c1991, 289p
See also PB92-148121 through PB92-148154 and See also PB92-148121 Infougn PB92-148184 and PB92-148063. Prepared in cooperation with American Inst. of Physics, New York. Sponsored by National Inst. of Standards and Technology, Gaithersburg, MD. Available from American Chemical Society, 1155 16th St., NW, Washington, DC. 20036-9976.

Keywords: \*Thermodynamic properties, \*Energy levels, Aluminum ions, Krypton ions, Oxygen, Water, Steam, Multicharged ions, Wavelengths, Tables(Data).

Wavelengths and Energy Level Classifications for the Spectra of Aluminum (Al 1 through Al XIII); Energy Levels of Krypton, Kr I through Kr XXXVI; Thermodynamic Properties of Oxygen from the Triple Point to 300 K with Pressures to 80

MPa; Sixteen Thousand Evaluated Experimental Thermodynamic Property Data for Water and

Cumulative Listing of Reprints and Supplements.

100,472 PB92-148121

(Order as PB92-148113) National Inst. of Standards and Technology, Gaithersburg, MD. Wavelengths and Energy Level Classifications for

the Spectra of Aluminum (All through Al XIII).

V. Kaufman, and W. C. Martin. c1991, 82p
Included in Jnl. of Physical and Chemical Reference

Data, v20 n5 p775-858 Sep/Oct 91. Available from American Chemical Society, 1155 16th St., NW, Washington, DC, 20036-9976.

Keywords: \*Aluminum ions, \*Aluminum, \*Energy levels, \*Wavelengths, Atomic energy levels, Atomic spectra, Multicharged ions, Positive ions, Tables(Data).

Wavelengths and their classifications have been compiled for the spectra of the atom and all positive ions of aluminum (Z=13). The selections of data are based on the compilations of energy levels by Martin and Zalubas (1970, J. Phys. Chem. Ref. Data 8, 817-864), with some updating from the more recent literature. Wavelengths (or wavenumbers) calculated from the differences of the energy levels are given, along with the observed values for all classified lines; these calculated wavelengths should in general be more accurate than the observed values wherever the two values differ significantly. Calculated wavelengths are also given for a number of lines that have not yet been observed, including some important forbidden transi-tions. The most complete data are given in separate tables for the different spectra. No limitation has been imposed on the wavelength range of the classified imposed on the wavelength range of the classified lines, except for the omission of x-ray transitions in the neutral atom. Two finding lists are also included, one for Al I through Al III and the other Al IV through Al XIII. (Copyright (c) 1991 by the U.S. Secretary of Commerce.)

100,473 PB92-148139

PB92-148139

(Order as PB92-148113)

National Inst. of Standards and Technology (PL),
Gaithersburg, MD. Atomic Physics Div.

Energy Levels of Krypton, Kr I through Kr XXXVI.

J. Sugar, and A. Musgrove. c1991, 57p

Sponsored by Department of Energy, Washington, DC.

Office of Magnetic Fusion Fnergy. Office of Magnetic Fusion Energy.

Included in Jnl. of Physical and Chemical Reference
Data, v20 n5 p859-915 Sep/Oct 91. Available from
American Chemical Society, 1155 16th St., NW, Wash-

ington, DC. 20036-9976. Keywords: \*Krypton ions, \*Krypton, \*Energy levels, Atomic energy levels, Multicharged ions, Ionized gases, Spectra, Tables(Data).

The energy levels of the krypton atom, in all stages of ionization for which experimental data are available, have been compiled. No data has yet been published for Kr XI through Kr XVII. For H-like krypton very accurate calculated level values are compiled. In all, data for 29 spectra are given. Experimental g-factors are included for Kr I and Kr II. Calculated percentage compositions of levels are given for 12 ions. A value for the ionization energy of each ion, either experimental or theoretical, is included. (Copyright (c) 1991 by the U.S. Secretary of Commerce.)

100,474 PB92-148147

(Order as PB92-148113)

Idaho Univ., Moscow. Thermodynamic Properties of Oxygen from the Triple Point to 300 K with Pressures to 80 MPa. R. B. Stewart, R. T. Jacobsen, and W. Wagner.

c1991, 105p Prepared in cooperation with Ruhr Univ., Bochum (Germany, F.R.). Inst. fuer Thermo- und Fluiddynamik. Included in Jnl. of Physical and Chemical Reference Data, v20 n5 p917-1021 Sep/Oct 91. Available from American Chemical Society, 1155 16th St., NW, Washington, DC. 20036-9976.

Keywords: \*Thermodynamic properties, \*Oxygen, Equations of state, Acoustic velocity, Specific heat, Enthalpy, Entropy, Density, Pressure dependence, Critical point, Triple point, Tables(Data).

A joint project by the authors has resulted in two new thermodynamic property formulations for oxygen. The fundamental equation explicit in Helmholtz energy by Schmidt and Wagner has been used for the calculation of the property tables presented here, and for comparisons of calculated properties to the experimental data. The formulation by Stewart and Jacobsen is used in the paper in comparisons of properties calculated by the two formulations. These comparisons provide the basis for independent assessment of the accuracy of the available data and calculated properties. The fundamental equation is valid for thermodynamic properties of oxygen from the freezing line to 300 K at pres-ties of oxygen from the freezing line to 300 K at pres-sures to 80 MPa. A separate vapor pressure equation and equations for the saturated liquid and saturated vapor densities and the ideal gas heat capacity are in-cluded. Functions for calculating internal energy, enthalpy, entropy, isochoric heat capacity (Cv), isobaric heat capacity (Cp) and velocity of sound are also included. Tables of thermodynamic properties of oxygen are given within the range of validity of the fundamental equation. The fundamental equation reported here may be used to calculate densities with an uncertainty of 0.10 percent, heat capacities within 2.0 percent, and velocity of sound values within 1.0 percent. These uncertainty values are valid for the range outside of the critical region. (Copyright (c) 1991 by the U.S. Secre tary of Commerce.)

100.475

PB92-148154

(Order as PB92-148113) Keio Univ., Yokohama (Japan). Dept. of Mechanical

Engineering Sixteen Thousand Evaluated Experimental Thermodynamic Property Data for Water and Steam. H. Sato, K. Watanabe, J. M. H. L. Sengers, J. S. Gallagher, and P. G. Hill. c1991, 22p

Gallagher, and P. G. Hill. c1991, 22p Prepared in cooperation with National Inst. of Standards and Technology (NML), Gaithersburg, MD. Thermophysics Div., British Columbia Univ., Vancouver. Dept. of Mechanical Engineering, Technische Univ. Muenchen (Germany, F.R.), and Ruhr Univ., Bochum (Germany, F.R.), Inst. fuer Thermo- und Fluiddynamik. Included in Jnl. of Physical and Chemical Reference Data, v20 n5 p1023-1044 Sep/Oct 91. Available from American Chemical Society, 1155 16th St., NW, Washington, DC. 20036-9976. ington, DC. 20036-9976.

Keywords: \*Thermodynamic properties, \*Steam tables(Thermodynamics), \*Water, Equation of state, Acoustic velocity, Vapor pressure, Metastable state, Pressure dependence, Density, Enthalpy, Virial coefficients of the properties of cients, Temperature dependence, Tables(Data).

As part of the activities of the International Association for the Properties of Water and Steam, all reliable sources of experimental data on the thermodynamic properties of ordinary (light) water and steam have been collected and converted to common temperature. ture, pressure, volume, mass and heat scales. The data are grouped by state or phase: ideal-gas properties; sublimation and melting curves; saturation properties; properties of liquid water at ambient pressure; thermodynamic properties of the single-phase state; and those of metastable states. In each category, a subdivision is made by property. Properties include the volume, enthalpy, heat capacities, sound velocity, internal energy and Joule-Thomson and related coefficients. cients. The total data collection contains approximately 16,000 data points and covers a century of experi-mental work at temperatures from 253 to 1273 K and pressures up to 1 GPa. The report characterizes the data and gives the literature references. The actual data collection is available in computerized form. (Copyright (c) 1991 by the U.S. Secretary of Commerce.)

100.476

PB92-148162 Not available NTIS American Chemical Society, Washington, DC.
Journal of Physical and Chemical Reference Data,
Volume 20, Number 6, November/December 1991.
Bimonthly rept.

Dill. Lide. c1991, 346p See also PB92-148170 through PB92-148220 and PB92-148113. Errata sheet inserted. Prepared in cooperation with American Inst. of Physics, New York.

Sponsored by National Inst. of Standards and Tech-

nology, Gaithersburg, MD. Available from American Chemical Society, 1155 16th St., NW, Washington, DC. 20036-9976.

Keywords: \*Physical chemistry, Atomic weights, Standards, Equations of State, Thermodynamic properties, Methane, Propulsion, Sulfuric acid, Carbon dioxide, Solubility, Reaction kinetics, High temperature tests, Combustion, Atmospheric chemistry, \*Foreign technology, Isotopic composition.

Contents:

A New Equation of State and Tables of Thermodynamic Properties for Methane Covering the Range from the Melting Line to 625 K at Pressures up to 1000 MPa;

Thermodynamic Properties of the Aqueous Sulfuric Acid System to 350 K; The Solubility of Carbon Dioxide in Water at Low

Pressure; Chemical Kinetic Data Sheets for High-Temperature Reactions. Part II; Atomic Weights of the Elements 1989; Isotopic Compositions of the Elements 1989.

# 100,477 PB92-148170

(Order as PB92-148162) Ruhr Univ., Bochum (Germany, F.R.). Inst. fuer Thermo- und Fluiddynamik.

New Equation of State and Tables of Thermody-

namic Properties for Methane Covering the Range from the Melting Line to 625 K at Pressures up to 1000 MPa.

U. Setzmann, and W. Wagner, c1991, 95p Included in Jnl. of Physical and Chemical Reference Data, v20 n6 p1061-1155 Nov/Dec 91. Available from American Chemical Society, 1155 16th St., NW, Washigton, DC 20036-9976.

Keywords: \*Equations of State, \*Thermodynamic properties, \*Methane, Tables(Data), Pressures, Specific heat, Helmholtz free energy, Enthalpy, Phase transformation, Ideal gas, Melting, Liquid-vapor interfaces, Saturation, Virial coefficients.

The work reviews the data on thermodynamic properties of methane which were available up to the middle of 1991 and presents a new equation of state in the form of a fundamental equation explicit in the Helm-holtz free energy. A new strategy for optimizing the structure of empirical thermodynamic correlation equations was used to determine the functional form of the equation. The Helmholtz function containing 40 fitted coefficients was fitted to selected experimental data of the following properties: (1) thermal properties of the single phase (P rho T) and (2) of the liquid-vapor saturation curve (P(sub s)rho' rho') including the Maxwell criterion, (3) speed of sound w, (4) isochoric heat capacity c upsilon, (5) isobaric heat capacity c(sub p), (6) difference of enthalpy delta h, and (7) second virial coefficient B. Independent equations are also included for the vapor pressure, the saturated liquid and vapor densities, the isobaric ideal gas heat capacity and the melting pressure as functions of temperature. Tables for the thermodynamic properties of methane from 90 K to 620 K for pressures up to 1000 MPa are presented. To verify the accuracy of the new formulation, the calculated property values are compared with selected experimental results and existing equations of state for methane. (Copyright (c) 1991 by the U.S. Secretary of Commerce.)

# 100,478 PB92-148188

(Order as PB92-148162) National Aeronautics and Space Administration, Cleveland, OH. Lewis Research Center.

Thermodynamic Properties of the Aqueous Sulfuric Acid System to 350 K.

Included in Jnl. of Physical and Chemical Reference Data, v20 n6 p1157-1200 Nov/Dec 91. Available from American Chemical Society, 1155 16th St., NW, Washington DC 20036 0075 ington, DC. 20036-9976.

Keywords: \*Thermodynamic properties, \*Sulfuric acid, Electrolytes, Liquid phases, Specific heat, Enthalpy, Melting points, Electromotive force, Tables(Data), Osmosis, Activity coefficients, Heat of fusion, Solid phases, Gibbs free energy, Freezing, Phase transformations, Entropy.

Experimental measurements for aqueous sulfuric acid and its related pure, solid phases have been thermodynamically analyzed and correlated as a function of temperature and composition from pure water to pure acid. The pure phases included anhydrous sulfuric acid, five of its hydrates and ice. Experimental data which were used in the correlation included measurements of the enthalpy of dilution, both solution and pure phase heat capacities, electromotive force and solution freezing points. The correlation yielded mutually consistent expressions for the Gibbs energy of each phase and these functions generally reproduce the experimental data to + or - 0.75 percent. The Gibbs energy functions of the pure solid phases were used to generate tables of their thermodynamic prop-erties from O K to the melting points. The Gibbs energy function for aqueous sulfuric acid was used to produce tables of both integral and partial molar solution properties as a sunction of sulfuric acid mole fraction every 50 degrees from 200 to 350 K. (Copyright (c) 1991 by the U.S. Secretary of Commerce.)

# 100,479 PB92-148196

(Order as PB92-148162) Alberta Univ., Edmonton. Dept of Chemical Engineer-

Solubility of Carbon DioxIde in Water at Low Pressure.

J. J. Carrol, J. D. Slupsky, and A. E. Mather. c1991,

Included in Jnl. of Physical and Chemical Reference Data, v20 n6 p1201-1209 Nov/Dec 91. Available from American Chemical Society, 1155 16th St., NW, Washington, DC, 20036-9976.

Keywords: \*Carbon dioxide, \*Solubility, Henrys law, Low pressure tests, Water, Enthalpy, Vapor phases, Chemical composition.

The system carbon dioxide-water is of great scientific and technological importance. Thus, it has been studied often. The literature for the solubility of carbon dioxide in water is vast and interdisciplinary. An exhaustive survey was conducted and approximately 100 experimental investigations were found that reported equilibrium data at pressures below 1 MPa. A model based on Henry's law was used to correlate the low pressure data (those up to 1 MPa). The following correlation of the Henry's constants (expressed on a mole fraction basis) was developed. In(H21/MPa) = -6.8346  $+\,$  12817/T-3766800/sq T  $+\,$  2.997 x 10 to the 8th power/cu T. The correlation is valid for 273 < T  $<\,$  433 K(0 < t < 160 C) where T is in K. Any experimental data that deviated significantly from this model were duly noted. (Copyright (c) 1991 by the U.S. Secretary of Commerce.)

# 100,480 PB92-148204

(Order as PB92-148162) Aerospace Corp., Los Angeles, CA. Chemical Kinetic Data Sheets for High-Temperature Reactions. Part 2. c1991, 100p

Included in Jnl. of Physical and Chemical Reference Data, v20 n6 p1211-1311 Nov/Dec 91. Available from American Chemical Society, 1155 16th St., NW, Washington, DC, 20036-9976.

Keywords: \*Reaction kinetics, \*High temperature tests, \*Combustion, \*Atmospheric chemistry, \*Propulsion, Vapor phases, Graphs(Charts), Thermochemistry, Oxygen atoms, Alkanes, Hydroxyl radicals, Halogen organic compounds, Oxygen, Ammonia.

Rate coefficient measurements for over fifty gasphase bimolecular reactions were critically evaluated and compared to theoretical calculations. The results of the work are summarized here in forty-nine Data Sheets, one sheet for each reaction or set of reactions of a single pair of reagents. The reactions chosen are of interest in propulsion, combustion, and atmospheric chemistry. Each Data Sheet consists of two pages that include a brief resume of the important experimental measurements and theoretical calculations, a graphical presentation of the data, a recommended rate coefficient expressed as a function of temperature, k(T) = AT(sup n) exp(-B/T), with probable uncertainty limits, a discussion of the basis for the recommendation, an equilibrium constant and a rate coefficient for the reverse reaction where applicable, and pertinent references. (Copyright (c) 1991 by the U.S. Secretary of Commerce.)

100,481 PB92-148212

(Order as PB92-148162)

Curtin Univ. of Technology, Bentley (Australia). Atomic Weights of the Elements 1989.

J. R. De Laeter, and K. G. Heumann. c1991, 13p Prepared in cooperation with Regensburg Univ. (Germany, F.R.).

Included in Jnl. of Physical and Chemical Reference Data, v20 n6 p1313-1325 Nov/Dec 91. Available from American Chemical Society, 1155 16th St., NW, Washington, DC. 20036-9976.

Keywords: \*Atomic weights, \*Standards, Chemical elements, Radioisotopes, Half life, Extraterrestrial matter, Tables(Data), Isotopic composition.

The biennial review of atomic weight, A(sub r)(E), determinations, and other cognate data has resulted in changes for nickel from  $58.69 + \text{or} \cdot 0.01$  to 58.6934 $\pm$  or - 0.0002 and for antimony from 121.75  $\pm$  or - 0.03 to 121.757  $\pm$  or - 0.003 due to new calibrated measurements. Because the measurement of the isotopic composition of mercury has also been improved during the last two years, the Commission was able to reduce the uncertainty of the atomic weight of this element from 200.59 + or - 0.03 to 200.59 + or - 0.02. Due to the nearly constant isotopic composition of protactinium in nature, where (231) Pa is the predominant isotope, the atomic weight of this element was fixed to 231.03588 + or - 0.000 02. The Table of Isotopic Compositions of the Elements 1989 will be published as a companion paper to that on Atomic Weights of the Elements 1989. The Table of Standard Atomic Weights Abridged to Five Significant Figures and current data on isotopic compositions of nonterrestrial material are included to benefit users who are more concerned with the length of time during which a given table has full validity to the precision limit of their interest. The Table of Atomic Weights to Four Significant Figures was prepared and has been published separately. (Copyright (c) 1991 by the U.S. Secretary of Commerce).

#### 100.482 PB92-148220

(Order as PB92-148162)

Curtin Univ. of Technology, Bentley (Australia). Isotopic Compositions of the Elements 1989. J. R. De Laeter, K. G. Heumann, and K. J. R.

Rosman, c1991, 11p Prepared in cooperation with Regensburg Univ. (Germany, F.R.).

Included in Jnl. of Physical and Chemical Reference Data, v20 n6 p1327-1337 Nov/Dec 91. Available from American Chemical Society, 1155 16th St., NW, Washington, DC. 20036-9976.

Keywords: Atomic weights, Chemical elements, Mass spectroscopy, Tables(Data), \*Isotopic composition.

The Subcommittee for Isotopic Abundance Measurements (SIAM) of the IUPAC Commission on Atomic Weights and Isotopic Abundances has carried out its biennial review of isotopic compositions, as determined by mass spectrometry and other relevant methods. The Subcommittee's critical evaluation of the published literature element by element forms the basis of the Table of Isotopic Compositions of the Elebasis of the Table of Isotopic Compositions of the Elements as Determined by Mass Spectrometry 1989, which is presented in the Report. Atomic Weights calculated from the tabulated isotopic abundances are consistent with A(sub r)(E) values listed in the Table of Standard Atomic Weights 1989. (Copyright (c) 1991 by the U.S. Secretary of Commerce).

### **Polymer Chemistry**

100.483 PB91-144402 PC A05/MF A01 National Inst. of Standards and Technology (NML), Boulder, CO. Chemical Engineering Science Div. Thermal Conductivity of a Polymide Film between 4.2 and 300 K, with and without Alumina Particles as Filler.

D. L. Rule, D. R. Smith, and L. L. Sparks. Aug 90, 77p NISTIR-3948

Sponsored by Ship Structure Committee, Washington,

Keywords: \*Polymeric films, \*Thermal conductivity, \*Composite materials, \*Polyimide resins, Ceramics, Polymer matrix composites, Aluminum oxide, Particles,

# **Polymer Chemistry**

Fillers, Cryogenics, Temperature dependence, Tables(Data), Graphs(Charts), Pressure dependence.

The thermal conductivity of several types of a commercial polyimide (specifically, polypyromellitimide: PPMI) film was measured over a range of temperatures from 4.2 to 300 K using an unguarded steady-state parallel-plate apparatus. Specimens were made by stacking multiple layers of film together. Conductive grease was used between layers of film to reduce there mal contact resistance. Two specimens were made mal contact resistance. Two specimens were made from two different types of neat (unadmixed) film with a thickness of 76 micrometers, and three specimens were made from films containing two different amounts of admixed alumina filler and having thicknesses of 25 micrometers or 76 micrometers. The concesses of 25 micrometers or 76 micrometers. The concesses of 25 micrometers or 76 micrometers. ductivity of PPMI film increases with the amount of alumina filler present. The thermal conductivity of specimens made from film of the same type but of different thickness is independent of film thickness, within the limits of experimental uncertainty. The thermal conductivity of a specimen subjected to a simulated curing process by being held at a temperature of 150 C for ninety minutes was indistinguishable from that of a similar, control specimen not subjected to such treatment.

100.484

PB91-147231 Not available NTIS National Bureau of Standards (IMSE), Gaithersburg, MD. Polymers Div.

Incorporation of Molecular Orientation into Systems of Lamellar Morphology. 1. Effects of Packing Entropy on the Lamellar Thickness of Block Copolymers.

Final rept.

E. A. DiMarzio. 1988, 8p Pub. in Macromolecules 21, n7 p2262-2269 Jul 88.

Keywords: \*Block copolymers, \*Entropy, \*Lamellar structure, Membranes, Orientation, Packing, Miceller systems, Molecular models, Thickness, Equations, Re-

Equations for the dimensions of the A and B regions of monodisperse diblock copolymers with lamellar morphology are obtained. An important feature of the treatment is the incorporation of the orientation-de-pendent packing entropy into the formalism. The equa-tions are believed to be accurate over the whole range of orientation of bonds, from random orientation to perfect alignment. Copolymer thicknesses vary as the 2/3 power of molecular weight to the first power depending on the amount of orientation induced by the packing entropy and the energetics. The amount of bond orientation in stretched molecules in bulk material is twice what the molecules would have if they were stretched (by the same stretch ratio) in solvent. It is observed that the effect is important to those systems of micelles, vesicles, membranes, soaps, liquid crystals, and block copolymers that experimentally are known to display significant orientation, and it is sug-gested that extant theories can be modified to include the effect.

100,485 PB91-148890 Not available NTIS National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Polymers Div. Chain Conformation of a Block Polymer in a Micro-

phase-Separated Structure.

Y. Matsushita, K. Mori, Y. Mogi, R. Saguchi, I. Noda, M. Nagasawa, T. Chang, C. Glinka, and C. Han.

Pub. in Macromolecules 23, n19 p4317-4321, 17 Sep

Keywords: \*Block copolymers, \*Polystyrene, \*Vinyl copolymers, \*Radius of gyration, Neutron scattering, Lamallar structure, Molecular weight, Pyridines, Measurement, Reprints.

The radii of gyration of a polystyrene block along the directions parallel and perpendicular to the lamellae in the lamellar structure of poly(styrene-b-2-vinylpyridine) were measured by small-angle neutron scattering. It was found that the block polymer is extended along the perpendicular direction, while it is contracted along the parallel direction. The extension is in accord with the theories of microphase-separated structure, but no theory predicts the contraction. From the molecular weight dependences of the radius of gyration along the directions parallel and perpendicular to the lamellae, it is concluded that the block polymer is contracted along the parallel direction to keep the volume occupied by the block chain constant when the microphase separation occurs.

100,486 PB91-158626 PB91-158626 Not available NTIS National Bureau of Standards (IMSE), Gaithersburg, MD. Polymers Div.

Measurement of Space Charge Fields in Polymers.

A. S. DeReggi, M. G. Broadhurst, G. T. Davis, and F. I. Mopsik. 1987, 6p Pub. in Proceedings of Annual Report Conference on Electrical Insulation and Dielectric Phenomena, Gaithersburg, MD., October 18-22, 1987, p307-312.

Keywords: \*Polymeric films, \*Electrical transients, \*Dielectric films, Pulses, Surface energy, Imbeddings(Mathematics), Electric fields, Electrodes, Laser heating, Polyethylene, Calibrating, Measurement, Laser heating, Space charge, Reprints, Ion-

Progress in analyzing and interpreting electrical transients induced by imbedded space charge when the surface of a dielectric polymer film is heated with short thermal pulses is reported. The thermal pulse currently comes from the energy of a dye laser absorbed by the electrodes. Measurement of the transient with and without a potential difference applied to the film allows (1) scaling and combining the transients obtained by heating each side of the film and (2) quantifying the resulting Fourier coefficients of the electric field distri-bution due to the imbedded space charge. The calibra-tion procedure is all electrical, and does not require a knowledge of the energy in the pulse, the electrode absorbency, or thermal properties of the polymer film.

100,487 PB91-159095 Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Chemical Engineering Science Div. Electrokinetic Demixing of Two-Phase Aqueous Polymer Systems. 1. Separation Rates of Polyeth-

ylene Glycol-Dextran Mixtures. Final rept. K. S. M. S. Raghava Rao, R. M. Stewart, and P. Todd. 1990, 12p

Pub. in Separation Science and Technology 25, n9-10 p985-996 1990.

Keywords: \*Separation processes, \*Solvent extraction, \*Electrophoresis, \*Polymers, Phase separation(Materials), Aqueous solutions, Electric fields, Buffers(Chemistry), Polyoxyethylene, Dextran, Polarity, Convection, Phosphates, Electrokinetics, Rates, Binary system(Materials), Reprints.

The separation of biomolecules and cells using aqueous two-phase systems provides a mild, nontoxic extraction medium, in contrast with conventional organicaqueous phase extraction. However, due to their similar physical properties, immiscible aqueous phases do not separate rapidly. Because a net surface potential occurs on phase droplets due to the unequal partitioning of certain dissolved ions, a study was undertaken in which the resulting motion in an electric field (electro-phoresis) was explored as a possible method for rapid demixing of aqueous two-phase systems in a vertical electrophoresis column. The effects of electric field strength, buffer concentration, and field polarity on the demixing rate of mixtures of polyethylene glycol and dextran in phosphate buffer were measured. It was found that an optimum field strength of around 29.2 V/cm exists at which demixing is most rapid and occurs at about twice the rate in zero field at 25 + or - 2C using normal polarity (anode at the top of the column). With reverse polarity (anode at the bottom; electric field opposing gravitational settling) at a field strength of 14.6 V/cm the rate was 3 times as fast as in zero field. Strong convection was observed at high field strengths. Increasing the phosphate concentration increased the demixing rate.

100,488 PB91-159715 PC A07/MF A01 National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Polymers Div.

Polymers: Technical Activities 1990.
L. E. Smith, and B. M. Fanconi. Jan 91, 134p See also PB86-165024.

Keywords: \*Polymers, \*US NBS, \*Research projects, Resins, Polymer matrix composites, Inks, Optical materials, Dental materials, Medical supplies, Biodeterioration, Injection molding, Process control, Mathematical models, Fluid flow, Mechanical properties, Polymer blends, Test equipment.

Technical Activities of the Polymers Division for FY 90 are reviewed. Included are descriptions of the 6 Tasks of the Division, project reports, publications, and other technical activities

100.489

PB91-162099 Not available NTIS National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Polymers Div.

Spinodal Decomposition in a Hydrogen-Bonded

Polymer Blend. Final rept.

M. He, Y. Liu, Y. Feng, M. Jiang, and C. C. Han. 1991, 10p Pub. in Macromolecules 24, n2 p464-473 1991.

Keywords: \*Polymer blends, Hydrogen bonds, Binary system(Materials), Polystyrne, Polyacrylates, Fluoropolymers, Opacity, Coarseness, Temperature measurement, Phase diagrams, Light scattering, Optical properties, Reprints, \*Spinodal decomposition.

The spinodal decomposition of a hydrogen-bonded binary blend, which consists of a polystyrene with 1.5 mol % of p-(1,1,1,3,3,3-hexafluoro-2-hydroxyisopro-pyl)-alpha-methylstyrene comonomer and a poly-(butyl psyl-apria-friethylstylene comonomer and a poly-fouty methacrylate), has been studied. The system has a LCST with a very asymmetrical phase diagram. Also the critical point does not coincide with the temperature minimum of either the spinodal or the cloud-point curve. The kinetics follows the Cahn-Hilliard-Cook model for early spinodal decomposition and a self-similar mechanism for late-stage coarsening for most cases. For shallow quench cases and for close to glass transition temperature cases, double peaks have been observed during spinodal decomposition, which suggests that a second or an alternative relaxation mechanism may be dominating the coarsening process. A special procedure has been developed to measure the cloud point for the system, which should be applicable to any polymer blend system that has a cloud temperature close to the glass transition temper-

100.490

PB91-162131 Not available NTIS National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Polymers Div. Time-Resolved Small-Angle Neutron Scattering in Intermediate- and Late-Stage Spinodal Decompo-

sition of (DPB/HPI) Blends.

Final rept. H. Jinnai, H. Hasegawa, T. Hashimoto, and C. C. Han. 1991, 8p

Pub. in Macromolecules 24, nl p282-289 1991.

Keywords: \*Polymer blends, \*Spinodal decomposition, Optical properties, Polyisoprene, Polybutadiene, Synthetic elastomers, Light scattering, Phase diagrams, Time resolution, Deuteration, Small angle scattering, Reprints.

Time-resolved small-angle neutron scattering (SANS) experiments were performed to study the later stage (i.e., the intermediate stage and the late stage) of spinodal decomposition (SD) of a critical mixture of perdeuterated polybutadiene (DPB) and protonated polyisoprene (HPI) with an LCST-type phase diagram and a critical temperature Te = 36.1 C Time-sliced SANS intensity, S(q,t), is generally composed of the scattering due to growing domains, I(sub d)(q,t), and that due to the thermally induced local composition fluctuations inside the domain I(sub tau)(q,t) where q and t are the scattering vector and time, respectively. S(q,t) as a function of q shows the 'spatial crossover' such that at q much below and above a time-dependent wavenumber, q(sub s)(t), it depends only on I(sub d)(q,t) and I(sub tau)(q,t), respectively. The time evolution of the composition difference between the two coexisting domains, delta phi(t), was determined from I(sub tau)(q,t), which was found to be consistent with the prediction of the scattering theory based upon the random-phase approximation. Delta phi(t) was found to increase with t and reach a constant equilibrium value delta phi(sub 0) at t>+(cr), where t(cr) is the crossover time from the intermediate to the late-stage SD. The crossover wavenumber, q(sub s)(t), also underwent a characteristic change at t(cr).

# **Polymer Chemistry**

100,491 PB91-162255 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Inorganic Analytical Research Div High Purity Fluoropolymer Materials: Trace Element Content and Leaching.

Final rept. J. R. Moody, E. S. Beary, D. S. Bushee, and P. J. Paulsen. 1988, 6p

Pub. in Jnl. of Crystal Growth 89, p43-48 1988.

Keywords: \*Fluoropolymers, Solvent extraction, Trace elements, Mass spectroscopy, Purification, Leaching, Crystal growth, Chemical analysis, Resins, Impurities,

Many problems in analytical chemistry are shared by the high purity crystal growth community since both are greatly concerned with the effects of impurities either upon an analysis or upon a device. Fluoropolymers are widely used today in applications where in-ertness or high purity or both are needed. The behavior of these polymers in high purity solvent systems has been investigated by several analytical techniques. Both the resin from which finished parts are made as well as blow molded bottles have been evaluated to determine cationic impurities in both the resin and in leachates.

100,492

PB91-174482 Not available NTIS National Bureau of Standards (IMSE), Gaithersburg, MD. Polymers Div.

Fluorescence Monitoring of Polymer Processing: Mixing and Zero Shear Viscosity.

Mixing and Zero Silear Viscosity.
Final rept.
A. Bur, F. Wang, and R. Lowry. 1988, 4p
Pub. in Proceedings of Society of Plastics Engineers
ANTEC '88, Atlanta, GA., April 18-22, 1988, p1107-

Keywords: \*Propellants, \*Polymers, \*Fluorescence spectroscopy, Process variables, Monitors, Temperature dependence, Doped materials, Mixing, Binders(Materials), Rheological properties, Reprints.

Fluorescence spectroscopy is being employed to monitor processing parameters such as non-Newtonian viscosity, molecular orientation, intersegmental penetration, and the degree of mixing of product ingredients. In order to do this, the processing ingredients are doped at a low concentration with fluorescent chromophores which are added as separate entities or chemically bound to the polymer binder. The chromophores are chosen in accordance with their sensitivity to a particular processing parameter. Information about the process being examined is obtained with the aid of known correlations between fluorescence spectra, rheological data, and other processing parameters. Two experiments determined: (1) the measurement of the change in fluorescence intensity as a function mixing time for a two component specimen, and (2) the measurement, at zero shear, of the dependence of the intensity of the fluorescence spectra from a doped polymer binder as a function of temperature. The feasibility of the fluorescence monitoring technique is demonstrated in each case.

Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Chemical Engineering Science Div. Statistical Mechanical Model of Aqueous Two-Phase Systems. Final rept.

H. Cabezas, J. D. Evans, and D. C. Szlag. 1989, 10p. Pub. in Fluid Phase Equilibria 53, p453-462 1989.

Keywords: \*Binary system(Materials), \*Polymer blends, Phase diagrams, Aqueous solutions, Statistical mechanics, Mathematical models, Forecasting, Interactions, Molecular weight, Polyoxyethylene, Dextran, Methyl cellulose, Virial coefficients, Reprints.

A predictive model for the phase diagrams of two-polymer aqueous two-phase systems has been developed from the solution theory of Hill. This theory gives chemical potentials in terms of isobaric isothermal osmotic virial coefficients representing polymer pair inter-actions. Predictive expressions for the dependence of these coefficients on molecular weight and polydispersity from Renormalization Group theory were developed. For a two-polymer system the model contains three monomer interaction coefficients, one for each polymer pair, and two scaling exponents, one for each polymer. Phase diagrams for four different systems have been calculated from the model at ambient conditions and shown to agree with experiment within 1-2% in polymer weight fraction. Two of the systems containpolyethylene glycol and dextran with molecular weights from 4000 to 280,000. The other two systems contain methylcellulose and dextran with molecular weights from 30,000 to 280,000.

100.494

PB91-187153 Not available NTIS National Inst. of Standards and Technology (IMSE),

Gaithersburg, MD. Polymers Div.
Small-Angle Neutron Scattering Studies of Compatible Blends of Linear Poly(Vinyl Methyl Ether) and Cross-Linked Deuterated Polystyrene. Final rept.

B. J. Bauer, R. M. Briber, and C. C. Han. 1989, 9p Pub. in Macromolecules 22, n2 p940-948 Feb 89.

Keywords: \*Polymer blends, \*Small angle scattering, \*Binary system(Materials), \*Vinyl ether resins, Phase separation(Materials), Networks, Temperature dependence, Crosslinking, Deuteration, Labeled substances, Graphs(Charts), Swelling, Reprints.

Small angle neutron scattering (SANS) from single phase polymer blends of crosslinked deuterated polystyrene (PSD) and linear polyvinylmethylether (PVME) has been studied as a function of temperature. Phase separation during the polymerization resulted if the PVME present is greater than the amount which would swell the PSD network at equilibrium, SANS from the single phase linear blend and the lowest crosslink density sample exhibited linear behavior for inverse zero angle scattering, 1/S(O) and inverse correlation length squared, 1/(xi)sup 2, versus 1/T while the higher crosslink density sample showed pronounced curvature in the same plot, eventually crossing over the curves for the other two samples. Linear plots for S(O) and xi versus 1/T for the highest crosslink density single phase sample could be obtained with the execution of the sample could be obtained with the execution. single phase sample could be obtained with the exponents 1/S(O)sup 57 and 1/(xi)sup 1.44 The highest crosslink density single phase sample was then de-formed to L/L=2.5 and the SANS examined as a function of temperature. The scattering obtained was an-isotropic with different values of S(O) and xi in the directions parallel and perpendicular to the deformation. Plots of 1/S(O) and 1/(xi)sup 2 versus 1/T indicated that the sample phase separated in the direction parallel to the deformation at a lower temperature than in the perpendicular direction.

100 495

Not available NTIS PB91-187229 National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Fire Measurement and Research

Molecular Dynamics Study of the Depolymerization Reaction in Simple Polymers. Final rept.

E. Blaisten-Barojas, and M. R. Nyden. 1990, 7p Sponsored by National Science Foundation, Washing-

Pub. in Chemical Physics Letters 171, n5-6 p499-505, 17 Aug 90.

Keywords: \*Depolymerization, \*Monomers, mistry), \*Combustion, Computerized \*Synthesis(Chemistry), \*Combustion, Computerized simulation, Reaction kinetics, Thermal degradation, Oxidation, Agglomerates, Infrared spectra, Temperature dependence, Reprints, \*Molecular dynamics.

A molecular dynamics experiment was designed to follow the sequence of depolymerization reactions occurring when a polymer degrades into its constituent monomers. The simulation addresses internal changes that certain materials undergo at the moment of burning. Polymer fragments were thermally generated from the random scission of longer polymer chains containing 50-950 units. Subsequently, these thermal fragments depolymerized and coiled dramatically, forming incipient 'agglomerates'. These agglomerates cooled while depolymerizing; the cooling mechanism remarkably inhibits the depolymerization reaction and eventually terminates the degradation process leading behind a sample of cold stable agglomerates. The size distribution of the polymer fragments is given as well as the IR spectrum of a typical sample at 2000 K.

100 496

PB91-187385 Not available NTIS National Inst. of Standards and Technology (IMSE), Gaithersburg, MD. Polymers Div.

Phenomenological Theory of the Influence of Strain History on the Rate of Isothermal Stress Relaxation.

Final rept. B. D. Coleman, and L. J. Zapas. 1989, 16p Pub. in Jnl. of Rheology 33, n3 p501-516 1989.

Keywords: \*Stress relaxation, \*Polymers, \*Strain \*Isotherms, Constitutive equations, Viscoelasticity, Theories, Time dependence, Rheological properties, Incompressible flow, Reprints, Strain history,

Constitutive relations are formulated for a class of incompressible viscoelastic fluids for which internal structural changes occur at a rate that is influenced by the history of the strain. For the materials considered, the contribution to the stress at time t made by the strain at an earlier time T is a function of that strain, the true elapsed time t - tau, and a quantity sigma (t, tau) that can be interpreted as the elapsed time measured by a clock whose rate of advance, because it is tied to the rate of structural change, is affected by the history of the strain. The functional relating delta sigma (t, tau)/delta t to the history of the strain up to time t is assumed to have the same domain and a structure similar to that relating stress to strain history. The present theory reduces to the theory of BKZ fluids in the (extreme) special case in which sigma (t, tau) = ttau, i.e., in which delta sigma (t, tau) delta t = 1. It is shown that there is a sense in which constitutive relations recently found to account well for observed discrepancies between experimental observations and predictions of the BKZ theory can be considered first-order approximations to the relations formulated here.

100,497 PB91-187427 Not available NTIS National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Polymers Div.

Multistep Stress-Relaxation Study of a Single Crystal of n-Eicosane (C20H42) in Torsion.

Final rept.

J. M. Crissman. 1989, 7p Pub. in Jnl. of Applied Physics 66, n1 p169-175, 1 Jul

Keywords: \*Single crystals, \*Stress relaxation, \*Polymers, Hydrocarbons, Viscoelasticity, Constitutive equations, Torsion tests, Time dependence, Reprints, Eicosane.

Multistep stress-relaxation experiments in torsion have been done on a single crystal of the long chain hydrocarbon compound n-eicosane. It was found that at very small strains the behavior approaches that of a linear viscoelastic material whereas at larger strains the behavior becomes increasingly nonlinear and time dependent. In the region where the stress-strain behavior becomes nonlinear it is shown that the second step response, in an experiment in which the magnitude of the second step is one half that of the first step, can be described very well using a recent constitutive equation derived by Zapas.

100.498

PB91-187450 Not available NTIS National Inst. of Standards and Technology (IMSE), Gaithersburg, MD. Polymers Div.
Statistics of a Polymer Molecule in the Presence of Asymmetric Obstacles.

Final rept.

E. A. Di Marzio. 1991, 10p Pub. in Macromolecules 24, n7 p1595-1604 1991.

Keywords: \*Polymers, \*Stereochemistry, \*Statistical analysis, \*Statistical mechanics, Configuration, Molecular weight, Barriers, Orientation, Chemical bonds, Probability, Reprints.

The number of configurations W of a polymer in a field of fixed obstacles is obtained. The cubic lattice of N sites has a coordination number z and is of d = z/2dimensions. The obstacles are modeled as rigid rods or rigid but bent polymers. A fraction of the obstacle bonds are oriented in orientation i. The flexible polymer which is placed into the field of rigid obstacles is of length M and has beta(sub i) of its bonds lying in orientation i. The formula for W results in expectation values only a few percent different from the exact expressions for the known special cases. The beta(sub i) are not fixed numbers but rather occur with a probability given by W. With the maximum term method the dimensions of the polymer are calculated. The polymer is elongated in the direction of alignment of the obsta-

# **Polymer Chemistry**

cles. The volume of the polymer is found to increase with volume fraction of obstacles for isotropically ordered obstacles, but it decreases for high concentrations of obstacles if the obstacles are strongly aligned. The scaling law exponent describing molecular weight dependence of linear polymer dimension is 0.6 for each of the three dimensions but deviates from the value for large elongation. Seven possible applications of the formula are discussed.

100,499 PB91-194456 PC A03/MF A01 National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Polymers Div.
Synthesis of Non-Ionic Water-Dispersible Resins

for Use in Intaglio Inks Curing by Electron Beam Radiation.

Annual rept.

B. Dickens, B. J. Bauer, and W. J. Pummer. May 91, 27p NISTIR-4564

Sponsored by Bureau of Engraving and Printing, Washington, DC.

Keywords: \*Inks, Aqueous solutions, Resins, Polymeric films, Radiation curing, Electron beams, Polymeriza-tion, Engraving, Printing, Chemical radiation effects, Polyethylene glycols, Methacrylates, Siloxanes, Phos-phazene, PMMA, Polyurethanes, Isocyanates, Viscosity, Synthesis(Chemistry), \*Intaglio.

Several types of non-ionic resins which cure under the action of radiation such as UV or electron beam have been synthesized. The resins disperse in neutral water when uncured. The water dispersibility is conferred by incorporating polyethylene oxide sequences in the resin molecules. The polymerizing action is conferred by methacrylate groups. Typically, one end of each polyethylene sequence is attached to a methacrylate group, and the other end is chemically linked in various ways to produce resins varying from 2 to 4 methacry-late functionality. The linking moieties used are (1) a phosphazene ring, (2) a siloxane center, (3) a poly (methyl methacrylate backbone, and (4) a mixture of difunctional and trifunctional isocyantes. When the resins containing the urethane linkages were used with low viscosity crosslinkers, the mixtures were of appro-priate viscosity for use in intaglio inks and cured with less than two megarads exposure to give reasonably flexible scuff-free films. The other resins were not vis-cous enough for use in intaglio inks and in some cases cured too slowly.

100,500 PB91-194688 Not available NTIS National Inst. of Standards and Technology (MSEL),

Gaithersburg, MD. Polymers Div.
Small-Angle Neutron Scattering of Blends of Cross-Linked and Linear Polystyrene.

Final rept. R. M. Briber, and B. J. Bauer. 1991, 6p Pub. in Macromolecules 24, n8 p1899-1904, 15 Apr

Keywords: \*Small angle scattering, \*Neutron, \*Polymer blends, \*Polystyrene, Labeled substances, Crosslinking, Networks, Thermodynamic properties, Deuteration, Isotope exchange, Synthesis(Chemistry), Divinylbenzene, Elastic properties, Free energy, Phase separation(Materials), Binary system(Materials), Density(Mass/volume), Mixing, Rubber, Reprints.

Small-angle neutron scattering (SANS) has been used to study the scattering function and thermodynamics of blends of linear protonated polystyrene (PSH) and cross-linked deuterated polystyrene (PSD). Two series of samples were synthesized. In both cases the sam-ples were made by dissolving the linear PSH in deuterated (d8) styrene monomer containing a small amount of divinylbenzene, which was then polymerized to form the PSD network around the linear PSH chains. The samples were all made at a concentration of 50/50 by weight PSD/PSH. Series 1 is a set of samples with the same cross-link density varying the length of the linear chain. Series 2 is a set of samples containing the same length linear chain varying the cross-link density systematically. By extrapolation of S(q) obtained from SANS using an Ornstien-Zernike plot (1/S(q) versus q squared) to q = 0, the zero-angle scattering, S(0), was obtained. S(0) is inversely proportional to the second derivative of the free energy with respect to composition. For the series 1 and 2 samples it was found that the samples could be driven to phase separation by increasing either the length of the linear chain or the network density. In the series 1 samples the zero-angle scattering scaled as 1/S(0) approximately=1/ N(sub b). In the series 2 samples the zero-angle scat-

tering scaled as 1/S(0)approximately=1/N(sub c). In addition, the scattering was found to increase as N(sub c) decreased for the series 2 samples, a behavior opposite to that predicted by combining classical rubber elasticity and mixing theories.

PB91-195099 Not available NTIS National Bureau of Standards (IMSE), Gaithersburg, MD. Polymers Div.

Relaxation of Crosslinked Networks: Theoretical Models and Apparent Power Law Behavior.

G. B. McKenna, and R. J. Gaylord. 1988, 6p Pub. in Polymer 29, n11 p2027-2032 Nov 88.

Keywords: \*Viscoelasticity, \*Relaxation, \*Synthetic elastomers, \*Crosslinking, Networks, Theories, Mathematical models, Density(Mass/Volume), Superposition(Mathematics), Time dependence, Reprints.

The viscoelastic behavior of crosslinked polymer networks is discussed. Models of the long term relaxation based on the retracing of dangling chains are described. It is pointed out that the theories all predict a power law time relation but differ in predictions of the crosslink density dependence of the power law exponent. The experimental data of Chasset and Thirion is examined. It is shown that the power law relation works only over a limited time span with deviations oc-curring at long times and more markedly for more highly crosslinked systems. Furthermore, the validity of time-crosslink density superposition for networks is confirmed, thereby precluding a crosslink density dependent exponent in any power law representation of the data.

100,502 PB91-195107 Not available NTIS National Inst. of Standards and Technology (IMSE),

Gaithersburg, MD. Polymers Div.
Study of the Linear Viscoelastic Properties of
Cyclic Polystyrenes Using Creep and Recovery Measurements.

Final rept. G. B. McKenna, B. J. Hostetter, N. Hadjichristidis, L. J. Fetters, and D. J. Plazek. 1989, 19p Pub. in Macromolecules 22, n4 p1834-1852 Apr 89.

Keywords: \*Polystyrene, \*Viscoelasticity, \*Molecular weight, "Rheological properties, \*Fractionation, Creep properties, Dilution, Measurement, Contamination, Cyclic compounds, Polymer blends, Chromatography, Reprints, Size exclusion chromatography, Zero shear viscosity, Recoverable compliance, Plateau compliance. Linear molecules.

The viscoelastic behavior of macrocyclic polystyrene fractions having molecular weights ranging from 19400 to 390000 was studied. Measurements of zero shear viscosity and recoverable compliance were made on the so-called Strasbourg fractions, Akron fractions, and two of the former which were refractionated. Also, studies of the effects of blending of up to 15.75% linear chains with the refractionated Strasbourg frac-tions were carried out. The studies show that the presence of linear chain contaminants in the macrocyclic fractions has the effect of decreasing the plateau compliance and increasing the steady state value of the recoverable compliance. Also, the presence of small amounts of linear contaminant increases dramatically the viscosity of the cyclic fractions. The results of analysis of the good and moderate fractions gives a picture of the cycles as showing 'classical' viscoelastic behavor the cycles as snowing classical viscoelastic behavior, i.e., the steady state recoverable compliance increases with increasing molecular weight and attains a constant value at high molecular weights (MW greater than 180,000), as do linear polymers. The zero shear viscosity-molecular weight relation is well described by an equation of the form viscosity = AM + BM(sup a) where a = 3.9, which is somewhat higher than the 3.4 power obtained for entangled linear chains. power obtained for entangled linear chains.

100.503 PB91-195271 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Fire Measurement and Research

Molecular Dynamics of Initial Events in the Thermal Degradation of Polymers.

Final rept. M. Nyden, and D. W. Noid. 1991, 6p Pub. in Jnl. of Physical Chemistry 95, n2 p940-945

Keywords: \*Combustion, \*Polyethylene, \*Thermal degradation, Polymers, Computerized simulation, Reaction kinetics, Mechanisms, Chemical bonds, Hydrogen bonds, Mathematical models, Reprints, \*Molecular dynamics.

Computer simulations, based on molecular dynamics, have been used to reveal kinetic and mechanistic aspects of initial events in the thermal degradation of polyethylene and related polymers. Simulations were performed on a series of model polymers and the rate constants for random scission of the carbon-carbon bonds were computed. The results are consistent with the predictions of statistical theories of unimolecular reactivity. Observations of the detailed motions of the model polymers have also revealed pronounced coiling actions in the vicinity of dissociating bonds. The behavior is examined in the light of proposed mechanisms for intramolecular hydrogen transfer.

100 504

PB91-195685 Not available NTIS National Inst. of Standards and Technology (IMSE), Gaithersburg, MD. Polymers Div. Difunctional and Multifunctional Monomers Capa-

ble of Cyclopolymerization. Final rept.

J. W. Stansbury. 1991, 7p Sponsored by National Inst. of Dental Research, Bethesda, MD.

Pub. in Macromolecules 24, n8 p2029-2035 1991.

Keywords: \*Acrylates, \*Esters, \*Cyclic compounds, \*Monomers, \*Polymerization, Synthesis(Chemistry), Aldehyde polymers, Dental materials, Ethers, Reaction kinetics, Steric hindrance, Solubility, Oligomers, Reprints, Diazabicyclooctane.

The reaction of an acrylate ester with paraformaldehyde in the presence of diazabicyclo(2.2.2)octane has been shown to provide access to novel ether-fused di-methacrylate-like monomers that can undergo cyclopolymerization. The study examined the influence of the pendant ester functionality on the synthesis and polymerization of these monomers. While bulky ester groups were generally found to reduce the rate of reaction in monomer synthesis, the more hindered monomers appear to polymerize through the available in-tramolecular cyclization pathway with greater efficiency than monomers without significant steric con-straints. Polymerizations in solution lead to mainly cy-clized, soluble polymers up to relatively high monomer concentrations. Bulk polymerizations provided brittle, cross-linked polymers with high degrees of conver-sion. The work was extended to include the synthesis of a multifunctional oligomer based on the same 1,6-diene substructure. The polymerization of this oli-gomer produced a tough, highly cross-linked polymer.

100.505 PB91-202887 Not available NTIS National Inst. of Standards and Technology (IMSE), Gaithershura MD. Palimera Discontinuous (IMSE), Gaithersburg, MD. Polymers Div.

Examination of Mechanisms Responsible for Incoherent Scattering of Subthermal Neutrons by Polymers.

L. D. Coyne, and W. L. Wu. 1989, 3p Pub. in Polymer Communications 30, n10 p312-314

Keywords: \*Small angle scattering, \*Thermal neutrons, \*PMMA, \*Polymers, Incoherent scattering, Mechanism, Neutron cross sections, Deuteration, Polyvinyl alcohol, Quantitative analysis, Methyl radicals, Methylene radicals, Hydroxy compounds, Glass transition temperature, Protons, Labelled compounds, Reprints, Methyne compounds.

Proper account for the large incoherent contribution is vital for quantitative evaluation of small-angle neutron scattering data of polymers. Knowledge of the relative contributions of hydrogen atoms in differing chemical substituents will aid in a priori estimates of incoherent scattering cross-sections for polymers of complex structure. From subthermal neutron transmission measurements on poly(methyl methacrylate) and hydrogenous and partially deuterated poly(vinyl alcohol) it is established that contributions to levels of incoherent scattering by protons in polymers are ordered quantitatively as -CH3>-OH>-CH2-,=CH-. No appar-ent effect of the glass transition on incoherent scattering of subthermal neutrons by polymers was dis-

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100,506 PB91-203224 Not available NTIS National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Polymers Div.

Morphology of Polymer Films and Single Molecules.

Final rept.

B. Howell, and D. H. Reneker. 1990, 20p Pub. in Jnl. of Applied Polymer Science 40, n9-10 p1663-1682 1990.

Keywords: \*Monomolecular films, \*Polymeric films, \*Plastics, \*Polystyrene, Labelled compounds, Electron microscopy, Thin films, Molecular weight, Peek, Polyethylene, Elastomers, Deuteration, PMMA, Block copolymers, Ruthenium oxide, Polyacetylenes, Polybutadiene, Glutamates, Reprints, Poly4BCMU, Polybutadiene, Glutamates, Reprints, Reprin benzyl-I-glutamate.

Seven polymeric substances were examined by high resolution electron microscopy. Features on the scale of the diameter of single molecular chains were observed. Polymers examined include: (1) linear polyethylene (Mw = 52,000), (2) polyethylene (Mw approximately 5,000,000), (3) poly-(cis-1,4-butadiene), (4) poly-gamma-benzyl-L-glutamate, polyetheretherketone) (PEEK), (6) deuterated polystyrene - poly(methylmethacrylate) (PMMA) block conductor and (2) polymer, and (7) a polydiacetylene, poly(1,12 di(butoxy-carbonylmethylurethanyl)-5,8-dodecadiyne), also called poly-4BCMU. A variety of methods were used to prepare dispersed single molecules, and very thin films, some of which had regions with strands containing only a few molecules. Staining with RuO4 revealed structures near the surface of the films that were reproducible and characteristic of each polymer.

100,507 PB91-203364 Not available NTIS National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Polymers Div.
Simulation Studies of Excluded Volume Effects on

Polymer Chain Dynamics in Several Nonlattice Models.

Final rept.

D. Kranbuehl, D. Eichinger, and P. H. Verdier. 1991,

Pub. in Macromolecules 24, n9 p2419-2427 1991.

Keywords: \*Polymers, \*Monte Carlo method, \*Statistical mechanics, Stereochemistry, Computerized simulation, Mathematical models, Scale(Ratio), Relaxation time, Diffusion, Molecular chains, Reprints, Markov chains, Chain length, Excluded volume, Off lattice.

Computer simulations of off-lattice bead-stick models of polymer chains with a variety of move rules have been carried out to gauge the effect of these move rules on the dynamical behavior of the chains. Long relaxation times, translational diffusion constants, and mean-square end-to-end length for chains of from 9 to 99 beads, both with and without excluded volume, are reported. For several move rules the excluded volume constraints increase the chain-length dependence of the long relaxation times by about the square root of chain length, roughly twice the exponent expected from simple scaling arguments based on the expansion of equilibrium dimensions by excluded volume. Move rules analogous to some of those used in the present study have been employed by others in previous lattice-model studies. Those earlier lattice-model results appeared to suggest that relaxation times scale like mean-square chain dimensions. Present results suggest, however, that the earlier result is an artifact resulting from the combination of lattice constraints with the use of move rules explicitly dependent upon local chain conformation.

100,508 PB91-203570 Not available NTIS

National Inst. of Standards and Technology (IMSE), Gaithersburg, MD. Polymers Div.
Tests of the Flory-Rehner Hypothesis: Comparison of the Elastic Free Energy Function for Crosslinked Rubber in the Dry and Swollen States.

G. B. McKenna, K. M. Flynn, and Y. Chen. 1989, 5p Pub. in Molecular Basis of Polymer Networks, p127-131 1989.

Keywords: \*Polymers, \*Solvents, \*Elastomers, \*Rubber, \*Free energy, \*Swelling, Networks, Elastic properties, Conformational changes, Compression tests, Torsion tests, Thermodynamic properties, Reprints, Frenkel-Flory-Rehner hypothesis.

One of the presumptions of the Frenkel-Flory-Rehner (FFR) hypothesis is that the form of the elastic component of the free energy function is not affected by the presence of solvent molecules. The change in elastic properties of the swollen rubber are then attributed to changes in chain conformation alone. Experiments in which the derivative of the elastic free energy with respect to the deformation for both dry and swollen rubber was measured were used to test the aspect of the FFR hypothesis. Torsional and compression experiments were carried out on samples of dicumyl peroxide crosslinked natural rubber. Results show that the elastic free energy function of a rubber network is unaffected, at least to first order, by the presence of solvent. This appears to be true over the entire range of experimental parameters investigated, i.e., crosslink density, solvent quality, and degree of swelling.

PB91-203711 Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Building Materials Div.

Reflection/Absorption FTIR Spectral Characteris-

tics of Thin and Thick Crosslinked Epoxy Films on Steel Substrates.

Final rept.

T. Nguyen, D. Bentz, and W. Byrd. 1988, 5p Pub. in Proceedings of ACS Division of Polymeric Ma-terials Science and Engineering, Los Angeles, CA., September 26-30, 1988, v59 p459-463.

Keywords: \*Polymeric films, \*Epoxy resins, \*Steels, \*Coatings(Materials), Thickness, Crosslinking, Thin films, Spectrum analysis, Amines, Infrared spectra, Calculation methods, Fourier transformation, Theories, Transmission, Substrates, Absorptivity, Reflection, Comparative evaluation, Reprints.

The study examined, both theoretically and experimentally, band shapes of the reflection/absorption FTIR spectra of thin and thick crosslinked epoxy films on steel substrates. Amine-cured epoxy films of be-tween 10nm and 2.5um were spin coated on mechanically polished cold rolled steel samples, and reflection/absorption FTIR (RA-FTIR) spectra were taken at 84 degree angle of incidence using single reflection and parallel polarized light. The theoretical curves were calculated using Greenler's boundary-value equations for films on metals. For thin films, except for the broad and strong bands at 1510 and 1247 1/cm which shifted to higher frequency, other bands were similar to that obtained by the transmission technique. For micrometer films, numerous bands shifted to higher frequency and the bands at 1510 and 1247 1/cm distorted and split. The theory agreed well with experimental results for thin films. However, for micrometer thick films, although the theory correctly predicted distortion and splittings of strong bands, it underesti-mated the intensity of the splitted bands. Comparison between experimental data and theoretical calculations on the relationship between RA-FTIR band intensity and film thickness will also be discussed.

100 510 PB91-222612 PC A07/MF A02 National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Polymers Div. Assessment of the State-of-the-Art for Process

Monitoring Sensors for Polymer Composites.
D. Hunston, W. McDonough, B. Fanconi, F. Mopsik, F. Wang, F. Phelan, and M. Chang. 1 Jun 91, 145p NISTIR-4514

Keywords: \*Polymers, \*Ultrasonics, \*Dielectrics, \*Detectors, \*Spectroscopy, \*Optical scanners, Process control, Sensor characteristics, Composite materials, \*Process monitoring, Research and development.

A variety of techniques have been applied to monitoring the changes that occur in the resin during composite processing. The report identifies and analyzes those techniques that have the most promise for online application, namely: ultrasonic, dielectric, spectroscopic, and optical techniques. All these methods have advantages and disadvantages, and the best technique for a given application will depend strongly on the materials and processes involved. The report discusses these on-line monitoring techniques and compares them in the areas of measurement speed, sampling volume, sensitivity to different resins, effects of fiber type, resistance to the manufacturing environment, interpretation of the data, adaptability for other uses, and temperature capabilities. The most important comparison, however, concerns the research and development work that is needed to achieve the full potential of each technique in applications on the factory floor. Dielectric and ultrasonic methods have an advantage in this connection because commercial equipment designed for process monitoring is already available. The various spectroscopic and optical methods are generally in an earlier stage of development. The great potential inherent in these latter methods. however, makes it highly desirable to actively pursue their developments as well.

PB91-236638 Not available NTIS National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Polymers Div.

Semiempirical Theory of Relaxation: Concentrated Polymer Solution Dynamics.

Final rept.

J. F. Douglas, and J. B. Hubbard, 1991, 15p Pub. in Macromolecules 24, n11 p3163-3177, 27 May

Keywords: \*Polymers, \*Viscoelasticity, \*Stress relaxation, \*Glass, \*Melts, Diffusion, Molecular weight, Cluster model, Transport theory, Homogeneity, Viscosity, Reprints, Memory effects.

Classical models of viscoelasticity neglect memory effects arising from material inhomogeneity and cooperative molecular motion. These memory effects are modeled by using an integral equation approach in which physical arguments are employed to estimate the memory kernel. The model memory kernel de-pends on two parameters: beta, which is interpreted as a measure of material inhomogeneity, and phi, which is interpreted as a measure of cooperativity of molecular motion. Here the authors apply a relaxation model to polymer melt dynamics. An idealized 'cluster' model of stress relaxation in glasses is introduced to estimate beta. This model rationalizes well the observed stress relaxation of polymer glasses. A cluster model is also introduced to estimate the molecular weight dependence of the zero-shear rate viscosity and the diffusion coefficient of entangled polymers. For flexible polymers in three dimensions the viscosity molecular weight exponent ranges in the interval 3.3 to 3.7, depending on the strength of the excluded-volume inter-action. The diffusion coefficient molecular weight exponent in three dimensions is predicted to lie in the interval -2.3 to -2.5. Results similar to the reptation model are obtained in four dimensions, and the Rouse theory is recovered in the limit of infinite dimensionality. Estimates of the concentration dependence of entangled polymer solution transport properties are also

100.512

PB91-236653 Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Chemical Engineering Science Div. Thin and Composite High-Flux Membranes of Perfluorosulfonated Ion-Exchange Polymer. Final rept.

B. K. Dutta, D. Randolph, and S. K. Sikdar. 1990,

Pub. in Jnl. of Membrane Science 54, p51-61 1990.

Keywords: \*Perfluoro compounds, \*Sulfonic acids, \*Membrane transport, \*Polymeric films, \*Castings, Composite structures, Ion exchange materials, Curing, Amino acids, Permeability, Thin films, Electron microscopy, Mixtures, Glycine, Alanines, Separation processes, Reprints.

The techniques of casting thin and composite membranes of perfluorosulfonic acid polymer (PFSA) are reviewed. The thin PFSA membrane was prepared by a hot-casting method using an aqueous methanol solution with nonsolvents cyclohexanol and dimethylfor-mamide. The composite PFSA membrane was coldcast and subsequently cured at a higher temperature. Scanning electron micrographs showed the thin membrane to be asymmetric, whereas the composite membrane had a thin homogeneous polymer layer on the porous support. Permeation through the membranes was tested using several amino acids and their mix-tures as model permeants. It was found that mem-branes of both types provided higher fluxes than the commercial membrane of the same polymeric material. Permeation studies on amino acid mixtures using the composite membrane revealed that glycine permeated faster than either L-alanine or L-phenylalanine, and that glycine separation factors were higher for the composite PFSA membrane than for other polymeric membranes.

# **Polymer Chemistry**

100,513 PB91-236786 Not available NTIS Not available NTIS
National Inst. of Standards and Technology (CSTL),
Gaithersburg, MD. Process Measurements Div.
Small-Angle Neutron Scattering and Light Scattering Studies on the Miscibility of Protonated Polyisoprene/Deuterated Polybutadiene Blends.

Final rept. H. Hasegawa, S. Sakurai, M. Takenaka, T. Hashimoto, and C. C. Han. 1991, 7p Pub. in Macromolecules 24, n8 p1813-1819 1991.

Keywords: \*Synthetic elastomers, \*Polyisoprene, \*Polybutadiene, Polymer blends, Neutron scattering, Light scattering, Solubility, Isotope exchange, Protons, Deuterium, Hydrogen, Binary system(Materials), Small angle scattering, Mixtures, Phase diagrams, Fluid-fluid interactions, Reprints.

Binary mixtures of protonated polyisoprene and deuterated polybutadiene with particular microstructures exhibit an LCST-type phase behavior. Small-angle exhibit an LCST-type phase behavior. Small-angle neutron scattering (SANS) and time-resolved small-angle light scattering (SALS) techniques were employed to study the static and dynamic phase behavior of the mixtures. From the static study by SANS, binary interaction parameters and the phase diagram were obtained. The spinodal temperature at the critical blend composition obtained by the analysis of SANS profiles from the single-phase state was in good agreement with that obtained by the time-resolved SALS measurements. The component polymers are premeasurements. The component polymers are pre-pared by living anionic polymerization and hence have well-defined molecular characteristics. Therefore, this system is considered to be an excellent polymer mix-ture system for the study of the relationships between static and dynamic phase behaviors of the polymer mixture and the molecular parameters such as molecular weight, polydispersity, microstructure, etc.

100,514 PB91-237842 Not available NTIS National Inst. of Standards and Technology (IMSE), Gaithersburg, MD. Polymers Div. Network Structure in Epoxies. 6. The Growth Proc-

ess Investigated by Neutron Scattering. Final rept. W. L. Wu, W. Su, and B. J. Bauer. 1989, 5p See also PB88-195094.

Pub. in Polymer 30, n8 p1384-1388 1989. Keywords: \*Epoxy resins, Curing, Molecular structure, Molecular weight, Neutron scattering, Percolation, Re-

The curing process of epoxies in bulk prior to the gelation threshold was investigated using small angle neutron scattering. Both the radius of gyration and the molecular weight of the partially cured molecular network were measured at various extent of cure. Two curing agents with a difference in their functionality were included to elucidate the curing mechanism. The experimental results were interpreted in terms of the classi-cal Flory-Stockmayer theory in one case and the percolation theory for the other case.

100,515 PB92-110196

(Order as PB92-110162)

Tennessee Univ., Knoxville. Dept. of Chemistry.
Heat Capacity and Other Thermodynamic Properties of Linear Macromolecules. 10. Update of the ATHAS 1980 Data Bank. M. Varma-Nair, and B. Wunderlich. c1991, 56p

Prepared in cooperation with Oak Ridge National Lab.,

TN. Chemistry Div.
Included in Jnl. of Physical and Chemical Reference
Data, v20 n2 p349-404 Mar/Apr 91. Available from
American Chemical Society, 1155 16th St., NW, Washington December 1000000 ington, DC. 20036-9976.

Keywords: \*Specific heat, \*Thermodynamic properties, \*Polymers, Linear systems, Information systems, Gibbs free energy, Experimental design, Aromatic compounds, Tables(Data), \*Reference materials, ATHAS system.

The prior published ATHAS 1980 Data Bank of experimental heat capacities of linear macromolecules that included critically reviewed material on almost 100 polymers is updated. In addition, the data bank has been computerized so that future updates can be made continuously, and new print-outs or computer files will be available from the authors from 1990 on. (Copyright (c) 1991 by the U.S. Secretary of Com100.516
PB92-116284
PC A07/MF A02
National Inst. of Standards and Technology (MSEL),
Gaithersburg, MD.
Polymers: Technical Activities 1991. (NAS-NRC As-

sessment Panel, February 13-14, 1992). L. E. Smith, and B. M. Fanconi. Oct 91, 131p NISTIR-4696

See also PB91-159715.

Keywords: \*Polymers, \*Polymer matrix composites, \*Polymer blends, Medical supplies, Dental materials, Standards, On-line measurement systems, Technolostandards, Oriente measurement systems, recumony transfer, Shear, Phase separation(Materials), Dissimilar materials bonding, Corona discharges, Vinyl polymers, Rheological properties, Automobiles, Thin films, Computerized simulation, Neutron scattering, Biodegradation, Porcelain, US NIST, Standard Reference Materials

All of the Division's programs are described in the report, organized according to these six Groups. These Groups have made a number of significant accomplishments during the last year. Some of these are summarized below: A computer simulation was performed the program of the formed to model resin flow in liquid molding of the front end structure of a Ford Escort; A NIST/industry consortium has evolved for the purpose of developing inline measurement technology based on optical and fluorescence methods; A combined light scattering photometer/rheometer has been constructed to examine phase separation behavior of polymer blends and solutions under the influence of a simple shear field; A unique new tool has been developed to study the physics involved in the adhesion between a polymer and a solid surface like glass; The distribution of polarization in poly(vinylidene fluoride) poled by corona discharge rather than by contacting electrodes indicated positive charge injection near the surface: Proton spin diffusion results indicated domain sizes in poly(butylmethacrylate)/hydroxy modified polystyrene blends with minimum dimensions in the 6-10 nm range and stoichiometries of the order of 75/25; Novel, siloxane-containing difunctional and multifunctional vinyl monomers were prepared; The apparent 'shift' in polymer blend phase separation temperature, Tc, under shear flow has been interpreted with the mode-cousnear flow has been interpreted with the mode-coupling theory for mean-field polymer blend systems; The radial flow behavior was successfully predicted from measurements in unidirectional flow. An exposure technique that rapidly determines whether or not a polymer is biodegradable has been developed; Instrumentation has been set up and calibrated to measure the dielectric constant of thin polymer films at high electric fields; A viscoelastic model of stresses in porcelain-metal strips has been developed.

100,517 PB92-116698 Not available NTIS National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Polymers Div.
Flexible Polymer with Excluded Volume at an Inter-

acting Penetrable Surface of Variable Dimension: A Multiple epsilon Perturbation Theory. Final rept.

J. F. Douglas, and M. K. Kosmas. 1989, 8p Pub. in Macromolecules 22, n5 p2412-2419 May 89.

Keywords: \*Polymers, \*Surface properties, Perturbation theory, Calculation methods, Interactions, Renormalization, Reprints, \*Excluded volume.

Application of the renormalization group method to the perturbative treatment of surface ineracting polymers with excluded volume currently requires the surface dimension to be fixed. A multiple epsilon perturbation expansion method is proposed to circumvent the technical restriction. There are numerous potential applications of multiple epsilon perturbation theory (e.g. com-bined treatment of binary and ternary excluded volume interactions) which can be pursued once the internal consistency of the method is demonstrated in higher order calculations. The surface interaction model provides a good starting point for studying the multiple method because of the relative simplicity of the perturbative calculations which provide the input into the multiple epsilon renormalization group calculations. Another convenient aspect of the model is that the consistency of the multiple epsilon method can be checked against accurate results for the limits of each interaction (surface and excluded volume) alone and the combined interactions for the special case of a two dimensional surface.

100,518 PB92-117266

Not available NTIS

National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Polymers Div.

Microstructure Effects on the Lower Critical Solution Temperature Phase Behavior of Deuterated Polybutadiene and Protonated Polyisoprene Blends Studied by Small-Angle Neutron Scattering.

Final rept.

S. Sakurai, H. Jinnai, H. Hasegawa, T. Hashimoto, and C. C. Han. 1991, 5p

Pub. in Macromolecules 24, n17 p4839-4843 1991.

Keywords: \*Synthetic elastomers, \*Polymer blends, \*Neutron scattering, \*Polybutadiene, \*Polyisoprene, Binary system(Materials), Microstructure, Small angle scattering, Deuteration, Isotope exchange, Labelled compounds, Solubility, Solutions, Critical temperature, Phase diagrams, Vinyl polymers, separation(Materials), Randomness, Reprints.

The miscibility of a blend of protonated polyisoprene (HPI) with the 3,4-linkage microstructure in the range 7-15% and of deuterated polybutadiene (DPB) with the 1,2-linkage microstructure in the range 12-28% was studied by small-angle neutron scattering (SANS). It was found that all blends studied here show lower critical solution temperature (LCST) type phase behaviors; i.e., the phase separation occurs by raising the temperature. It was also found that the miscibility is quite sensitive to the microstructures of the polydienes used. The effective thermodynamic interaction parameter (chi(eff)) per segment between two polymers was determined by fitting SANS data in the single-phase state with a theoretical scattering curve obtained on the basis of the random-phase approximation. The temperature dependence of (chi(eff)) showed a systematic change with the microstructure. For a given HPI, the (chi(eff)) values decreased, and therefore, the blends became more miscible, with an increase in the vinyl content (i.e., 1,2-linkage content) in DPB. On the contrary, for a given DPB, the values increased, and therefore, the blends became more immiscible, with an increase in the vinyl content (i.e., 3,4-linkage content) in HPI. An alternative explanation for the LCST phase behavior is proposed based on treatment for the random copolymer blends.

100,519

PB92-117274 Not available NTIS National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Polymers Div.

Small-Angle Neutron Scattering and Light Scattering Study on the Miscibility of Poly(styrene-ran-butadiene)/Polybutadiene Blends.

Final rept.

S. Sakurai, T. Izumitani, H. Hasegawa, T. Hashimoto, and C. Han, 1991, 8p

See also PB91-236786.

Pub. in Macromolecules 24, n17 p4844-4851 1991.

Keywords: \*Solubility, \*Polymer blends, \*Synthetic elastomers, \*Styrene butadine resins, \*Polybutadiene, Binary system(Materials), Copolymers, Small angle scattering, Randomness, Light scattering, Neutron scattering, X-ray scattering, Predictions, Reprints.

The miscibility of binary blends of polybutadiene (PB) and poly(styrene-ran-butadiene)(SBR) was studied on the basis of segmental interaction parameters. In the analysis PB was assumed to be a random copolymer comprising 1,2-linkages (V) and 1,4-linkages (B) and SBR to be the one comprising styrene (S) and butadiene with V and B. The segmental interaction parameters between V and S (chi vs), B and S (chi bs), and V and B (chi vb) were determined on the basis of the copolymer blend theory from the effective interaction parameters (chi eff's) for the blends of PB and SBR, and those for poly(styrene-b-butadiene-b-styrene) triblock copolymer (SBS), with different copolymer compositions and microstructures of polybutadienes. The values chi eff wer determined from either the smallangle neutron or X-ray scattering of the mixtures in the single-phase state. By use of these segmental interaction parameters, chi vs, chi bs, and chi vb, the miscibility of the SBR/PB blends was predicted for a given set of V, B, and S contents in PB and SBR. The predictions of the miscibility for several SBR/PB blends agreed well with the results of the light scattering experiments.

#### General

100,520 PB92-112499 PC A04/MF A01 National Inst. of Standards and Technology (CSTL), Gaithersburg, MD. NIST Calibration Services for Humidity Measure-

A. Wexler, R. W. Hyland, S. Hasegawa, and P. H. Huang. Oct 91, 65p NISTIR-4677 See also PB270 049.

Keywords: \*Humidity measurement, \*Calibration, \*Hygrometers, Water vapor, Moisture content, Calibration standards, Gas generating systems, Vapor pressure, Error analysis, Tables(Data), US NIST.

The National Institute of Standards and Technology (NIST), formerly National Bureau of Standards (NBS), provides a service to Government agencies and the public for the calibration of humidity measuring instruments. Calibrations are performed by subjecting the instrument under test to atmospheres of known moisture content produced by the NBS two-pressure humidity generator. The most accurate calibrations are made with the NBS standard hygrometer, a device based on the gravimetric method. The internal report documents the original work for the NBS standard hygrometer, and for the NBS two-pressure humidity generator. The operations, tests, calibrations of component parts, and sources of errors of the standard hygrometer and the humidity generator are summarized. The random and systematic errors affecting the overall accuracy of the standard hygrometer and the humidity generator are analyzed and shown by tables.

# CIVIL ENGINEERING

# Construction Equipment, Materials, & Supplies

100,521 PB91-134189 Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Building Materials Div. Techniques to Observe the Fracture Zone in Mortar and Concrete.

Final rept. L. I. Knab, H. Jennings, H. N. Walker, J. R. Clifton,

and J. W. Grimes. 1986, 7p Pub. in Fracture Toughness and Fracture Energy of Concrete, p241-247 1986.

Keywords: \*Crack propagation, \*Concretes, \*Microscopy, Mortars(Material), Fractures(Materials), Electron microscopy, Fluorescence, Cracking(Fracturing), Fracture tests, Fracture zones, Building materials, Reprints.

There have been relatively few studies of the microstructural details of the fracture zone of propagating cracks in mortar and concrete. This lack of detailed information has hindered the development and validation of fracture mechanics theories based on the micromechanisms of crack propagation. The paper presents the application of two techniques to observe the microstructural details of the fracture zone: fluorescent light microscopy using thin sections, and scanning electron microscopy using backscattered electrons. Preliminary findings indicate that both techniques have the potential to provide new information on the fracture zone in mortar and concrete, both near the exterior and in the interior of specimens.

PC A04/MF A01 PB91-143321
PC A04/MF A01
National Inst. of Standards and Technology (NEL),
Gaithersburg, MD. Center for Building Technology.
Outline of a National Plan on High-Performance
Concrete: Report on the NIST/ACI Workshop. Held
in Gaithersburg, MD on May 16-18, 1990.
N. J. Carino, and J. R. Clifton. Dec 90, 63p NISTIR-

Keywords: \*High strength concretes, \*Meetings, Alkali aggregate reactions, Mechanical properties, Service life, Specifications, Concrete durability, Standards, Tests, Curing, Mixing, Recommendations.

A workshop on high-performance concrete (HPC) was held in Gaithersburg, MD on May 16, 17, and 18, 1990. The workshop was co-sponsored by the American Concrete Institute. High-performance concrete was defined as concrete having desired properties and uni-formity which cannot be obtained routinely using only conventional constituents and normal mixing, placing, and curing practices. Eight working groups were orga-nized to address different topics. The report summa-rizes the discussions and conclusions of the working groups. Each chapter begins with a brief introduction providing background on the nature of the problems addressed by the working group. Specific research topics are identified, and discussions are provided to explain the rationale for the needed research. The recommended research is proposed as the basis for a national program to exploit the potential of high-performance concrete and ensure U.S. competitiveness in concrete technology. Recommendations for implementing the plan are provided.

Not available NTIS PB91-148072 Mational Bureau of Standards (NEL), Gaithersburg, MD. Building Materials Div.

Microstructure and Fracture at the Cement Paste-

Aggregate Interface.

Final rept. L. Struble. 1988, 10p

Sponsored by Air Force Office of Scientific Research, Bolling AFB, DC. Pub. in Materials Research Society Symposium Pro-

ceedings, v114 p11-20 1988.

Keywords: \*Microstructure, \*Bonding strength, \*Cements, \*Aggregates, \*Fractures(Materials), Cementing, Interfaces, Cement aggregate reactions, Concretes, Bonding, Cracks, Reprints.

The mechanical behavior of concrete in thought to be affected by the microstructure of the paste-aggregate interface, which differs in several respects from the microstructure of bulk paste. General aspects of interfacial microstructure, which appear to be fairly well understood, are reviewed. Recent microstructural studies using back-scattered electron imaging show that there is a zone along the interface (approximately 50 micrometers wide) within which there are generally few large unhydrated clinker grains, many large voids (greater than 5 micrometers), a generally porous microstructure, many hollow-shell hydration grains, and in some cases little calcium hydroxide. The tendency for cracks to develop or grow along the paste-aggregate interface is discussed in relation to specific features of the interfacial microstructure.

100,524 PB91-148528 PC A03/MF A01 National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Center for Building Technology. Guide to the Use of the Cement and Concrete Re-search Remote Bulletin Board System (RBBS) Computer. L. J. Kaetzel, and J. R. Clifton. Dec 90, 49p NISTIR-

4473

Keywords: \*Cements, \*Concretes, \*Research projects, \*Data bases, Computer systems hardware, Information systems, Computer systems programs, Data transmission, Data retrieval, \*Remote bulletin board system, National Institute of Standards and Technology.

A computer system has been installed at the National Institute of Standards and Technology, Building Mate-rials Division, for exchanging and disseminating information related to cement and concrete research. The computer is accessible, remotely, through telephone lines. Messages, and computer stored files in many formats can be exchanged among cement researchers. Also, information can be retrieved and/or viewed that describes: scheduled symposia, archived computer based models, project summaries, and published papers. The document describes how to use the computer system.

Not available NTIS PB91-149922 National Bureau of Standards (NEL), Gaithersburg, MD. Building Materials Div.

Pozzolan Programs of the Cement and Concrete

Reference Laboratory. Final rept.

See also PB80-160047. Sponsored by American Society for Testing and Materials, Philadelphia, PA.

Pub. in Proceedings of the International Ash Utilization Symposium (8th), p19-1-19-13 1987.

Keywords: \*Laboratories, \*Concretes, \*Cements, Pozzolans, Aggregates, Inspection, Fly ash, Admixtures, Concrete durability, Standards, Quality assurance, Reprints.

The Cement and Concrete Reference Laboratory (CCRL) located in the Center for Building Technology of the National Bureau of Standards has as its goal the improvement in the quality of testing of construction materials. This is accomplished through the inspection of laboratories who test construction materials, distribution of proficiency samples, studies of testing prob-lems, and participation on technical committees. Until recently, the inspection and proficiency sample programs considered portland, blended and masonry cements; portland cement concrete; aggregates; and reinforcing steel. In response to requests of the Joint ASTM C1/C9 Subcommittee on the CCRL, two new programs related to pozzolans have been added; a pozzolan laboratory inspection program was begun in January 1987 and the distribution of a fly ash reference sample is planned for September 1987. The paper will provide a short overview of CCRL programs for cement, concrete, aggregates and reinforcing steel and give specifics on the pozzolan programs including scope of coverage, schedules, costs, anticipated benefits, and participation information.

100,526

PB91-174524 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Structures Div. Introduction to ACI 306.1-87: Specification for Cold Weather Concreting. Final rept. N. J. Carino. 1988, 8p Pub. in Concrete International 10, p50-57 Oct 88.

Keywords: \*Cold weather construction, \*Concrete construction, \*Specifications, Concrete durability, Structural forms, Concrete structures, Concretes, Freezing, Construction, Strength, Reprints.

The historical developments leading to the new ACI specification on cold weather concreting are reviewed. Attention is focused on the evolution of the current definition of 'cold weather' and on changes in the protection requirements to prevent damage from freezing at an early age. The evolution of the current criteria for form removal is also reviewed, and the paper concludes with a presentation of key aspects of the standard specification.

100,527

PB91-175117 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Structures Div. Rate Constant Functions for Strength Development of Concrete. Final rept.

R. C. Tank, and N. J. Carino. 1991, 10p Pub. in ACI Materials Jnl. 88, n1 p74-83 Jan/Feb 91.

Keywords: \*Concretes, \*Curing, \*Strength, Concrete construction, Temperature effects, Concrete durability, Mechanical properties, Aging tests(Materials), Con-struction materials, Concrete structures, structures. Life(Durability), Reprints.

The rate constant for strength development of a particular concrete mixture is the initial slope of the relative strength-versus-age curve at constant temperature curing. The form of the rate constant versus temperature function is needed to describe the combined effects of time and temperature on strength development. The study investigates the relationship between the rate constant and curing temperature. Based on strength gain data for concrete and mortar specimens made with Type I cement and cured at 10, 23, and 40 C (50, 73, and 104 F), the following conclusions are drawn: (1) strength gain can be represented by a three-parameter hyperbolic function; (2) the rate constant is a nonlinear function of curing temperature and a simple exponential function describes the relationship; (3) tests of appropriate mortar specimens provide the information needed to predict relative strength de-velopment of the corresponding concrete; and (4) the proposed rate constant model accurately describes the development of relative strength as a function of the equivalent age.

### CIVIL ENGINEERING

# Construction Equipment, Materials, & Supplies

100,528 PB91-178863 PC A03/MF A01 National Inst. of Standards and Technology (BFRL), Gaithersburg, MD. Characterization of Field Concrete. P. E. Stutzman. Jan 91, 35p NISTIR-4516

Keywords: \*Concretes, \*Field tests, Construction materials, Performance prediction, Service life, Chemical analysis, Characterization, Crack propagation, Microstructure, Compressive strength, Sampling, Tests.

Field inspection and laboratory analysis of concrete and concrete structures are necessary for condition evaluation, determination of the need and extent of re-pairs, and for the prediction of concrete service life. A detailed evaluation includes field inspection, field testing, sampling, and laboratory analyses and also involves the description of the structure, concrete, and aggregates. Field inspection for overall structure condition includes the identification and description of surface defects, cracks, and cracking patterns. Field test-ing determines relative concrete quality and location of degraded concrete, and provides guidance in developing a sampling plan. Laboratory analyses provide detailed information on the microstructure, phase composition, chemical composition, and strength of the concrete.

100 529 PB91-187179 Not available NTIS National Inst. of Standards and Technology (NEL),

Gaithersburg, MD. Building Materials Div.

Percolation of Phases in a Three-Dimensional Cement Paste Microstructural Model.

Final rept. D. P. Bentz, and E. J. Garboczi. 1991, 20p Sponsored by National Science Foundation, Washington, DC.

Pub. in Cement and Concrete Research 21, p325-344 1991

Keywords: \*Cements, \*Microstructure, \*Hydration, \*Percolation, Water cement ratio, Admixtures, Porosity, Curing, Computerized simulation, Models, Reprints.

A three-dimensional digital-image-based simulation model of cement hydration is used to study the percolation or connectivity of phases as a function of hydration. Results from an investigation of the effects of water-to-cement ratio, degree of hydration, and the substitution of inert and pozzolanic mineral admixtures for cement, on the connectivity of the capillary porosity are presented. For all scenarios studied, plotting pore connectivity vs. total porosity results in a single universal curve. Based on the curve, the degree of hydration required to achieve pore discontinuity as a function of water-to-cement ratio and pozzolanic mineral admixture concentration has been determined. Similar universal curves have been obtained for the connectivity of the calcium silicate hydrate and calcium hydroxide phases in hydrated neat cement when plotted against the appropriate phase fraction. Simulation results are analyzed using percolation theory, and are applied to interpreting observed experimental results concerning cement properties as a function of hydration.

100.530 PB91-189621 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Building Materials Div.

Evaluation of Test Methods for Measuring the Bond Strength of Portland Cement-Based Repair

Materials to Concrete.

Final rept.

L. I. Knab, and C. Spring. 1989, 12p See also PB88-215488. Sponsored by Tri-Service Building Materials Committee, Washington, DC. Pub. in Cement, Concrete and Aggregates 11, n1 p3-14 1989.

Keywords: \*Portland cements, \*Bonding strength, Tension tests, Tensile stress, Repair, Bonding, Mechanical properties, Dissimilar materials bonding, Concretes, Tensile strength, Concrete construction, Re-

Three bond test methods were evaluated for screening and selecting repair materials used in overlaying and patching portland cement concrete. The bond strengths of three repair materials to base concrete were investigated using two uniaxial tensile bond test methods and a slant shear bond test method. The differing strength characteristics of the repair materials as compared to the base concrete resulted in different

failure patterns, which had to be taken into account in the analyses of the failure stresses. Substantial differences in the failure stresses of the two test types (slant shear and uniaxial tension) were attributed to their completely different geometries and loading condi-tions. Differences in the failure stress of the two test types emphasized the importance of selecting a test method that simulates, in so far as possible, the anticipated in-service conditions of repair material. It was concluded that both the slant shear test method and the pipe nipple grips uniaxial tensile test method can be used to screen and select repair materials of the type investigated (portland cement concrete or latex modified concrete) for overlaying or patching portland cement concrete.

100.531

PB91-203836 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Building Materials Div. Activities of the Construction Materials Reference Laboratories Related to Laboratory Accreditation. Final rept. J. H. Pielert. 1989, 7p Sponsored by American Association of State Highway

nd Transportation Officials, Washington, DC Pub. in Accreditation Practices for Inspections, Tests, and Laboratories, ASTM STP 1057, p30-36 1989.

Keywords: \*Construction materials, Test facilities, Aggregates, Concretes, Standards, Reprints, \*Laboratory accreditation.

conference was held at the National Institute of Standards and Technology (formerly The National Bureau of Standards) in May 1986 to consider the status of existing evaluation and accreditation programs for construction materials testing laboratories and to determine the need for a coordinated national system. The conference attendees concluded that there is a need for a coordinated national system for the accreditation of construction materials testing lab-oratories and its development should be initiated.' The paper will discuss activities since the conference, including the work of a planning committee formed to define the goals, scope, format, and procedures of such a system. There will be particular emphasis on activities of CCRL and AMRL, which make up the Construction Materials Reference Laboratories. They are research associate programs at NIST sponsored by ASTM and AASHTO, respectively, and provide labora-ASTM and AASHTO, respectively, and provide labora-tory assessment and proficiency sample services, but do not accredit laboratories. However, the AASHTO Executive and Policy Committee approved the AASHTO Accreditation Program utilizing AMRL techni-cal programs for implementation in mid-1988. The Ex-ecutive Group of the Joint ASTM C1/C9 Subcommit-tee on the CCRL is changing CCRL programs for con-crete and concrete agreeates to expely with procrete and concrete aggregates to comply with new ASTM laboratory evaluation standards.

100.532 PB91-240804 PC A03/MF A01 National Inst. of Standards and Technology (BFRL), Gaithersburg, MD.
Guidelines for the Development of Computer Based Models in a Cementitious Materials Model-

ing Laboratory.
L. J. Kaetzel, J. R. Clifton, and L. J. Struble. Aug 91, 35p NISTIR-4650

Prepared in cooperation with Illinois Univ. at Urbana-Champaign. Dept. of Civil Engineering.

Keywords: \*Cements, \*Materials tests, \*Mathematical models, \*Computerized simulation, Construction materials, US NBS, Software engineering, Recommendations, Standards, National science Foundation, Data bases, Equipment interfaces, Computer networks.

The paper presents guidelines and considerations for the development, archiving, and distribution of com-puter models for a centralized cementitious materials modeling laboratory. An analysis of the approach used by cement researchers to develop large complex com-puter models reveals the need for guidelines in selecting computer platforms, software languages and tools, software engineering and documentation. A modeling laboratory established at NIST associated with the NSF Center for Science and Technology of Advanced Cement-Based Materials is discussed and the important of such a facility in promoting the exchange of in-formation (i.e. ideas, models, data). The computer models currently archived in the modeling laboratory are used as test cases to describe the facility.

100.533

PB92-116300 PC A03/MF A01 National Inst. of Standards and Technology (BFRL), Gaithersburg, MD.

Uniaxial Tensile Tests to Measure the Bond of In situ Concrete Overlays. R. G. Mathey, and L. I. Knab. Oct 91, 37p NISTIR-

4648

See also PB90-204520, Sponsored by U.S. Army Corps of Engineers, Washington, DC, Naval Facilities Engineering Command, Alexandria, VA, Air Force Engineering and Services, AFB, Washington, DC.

Keywords: \*Pavement overlays, \*Concrete pavements, \*Bonding strength, \*Tension tests, Tensile properties, Concrete slabs, Dissimilar materials bonding, Concretes, Mechanical properties, Tensile strength, Concrete durability, Test facilities, Mechani-

The feasibility of two in situ tensile test methods for use in the field to measure the bond of concrete overlays was investigated in the laboratory. The two test methods used pneumatic and hydraulic loading apparatuses. The uniaxial tensile tests were conducted using partial-depth in situ cores drilled through overlay concrete and into previously cast slabs. Comparisons of the magnitude and repeatability of the tensile strength results for the two test methods indicated that they were comparable. The study demonstrated that both the pneumatic and hydraulic test methods are applicable for field use for measuring the tensile strength of the bond between a relatively thick overlay and its base concrete.

# **Highway Engineering**

PB91-187849 PC A04/MF A01 National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Center for Building Technology. Proposed Design Criteria for Shallow Bridge Foundations.

F. Y. Yokel. Feb 90, 57p NISTIR-90/4248 Sponsored by Federal Highway Administration, McLean, VA. Office of Research, Development, and Technology.

Keywords: \*Bridge foundations, \*Design criteria, \*Settlement(Structural), Loads(Forces), Structural engineering, Highway bridges, Displacement, Bearing capacity, Ultimate strength, Failure, Stresses.

Criteria for the design of spread footings for highway bridges are proposed. The criteria address working load as well as load and resistance factor design (LRFD) procedures. Importance factors to be used in conjunction with the LRFD design format are proposed. The importance factors increase the design loads as the span length increases and also otherwise account for the severity of the consequences of a structural or foundation failure. Further data on LRFD design will be available from studies presently in progress. Available information on tolerances of highway bridges and other structures to foundation displacements are reviewed. On the basis of the information, allowable foundation-displacement limits are proposed. Unconditionally allowable foundation displacements will not affect the strength and serviceability of bridges and therefore do not require structural design modifications.

# COMBUSTION, **ENGINES, & PROPELLANTS**

### Combustion & Ignition

PB91-134510 Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Fire Measurement and Research Div. Aspects of Smoldering Combustion.

Final rept. T. J. Ohlemiller. 1987, 9p

Pub. in Proceedings of International Conference on the Physical and Chemical Processes Occurring in a Burning Cigarette, Winston-Salem, NC., April 26-29, 1987, p346-354.

Keywords: \*Combustion, Reprints, \*Cigarettes, Fire models.

Several application areas of smoldering combustion phenomena are reviewed and inter-compared to dem-onstrate the range of length and time scales possible, as well as the dependence of controlling factors on the configuration of the smolder wave. Existing models for these same application areas are briefly examined.

PB91-144428 PC A04/MF A01 National Inst. of Standards and Technology (NML), Boulder, CO. Chemical Engineering Science Div. Ignition Characteristics of the Nickel-Based Alloy UNS N07001 in Pressurized Oxygen.

J. W. Bransford, and P. A. Billiard. Sep 90, 53p NISTIR-3947

Prepared in cooperation with Boeing Co., Seattle, WA. Sponsored by National Aeronautics and Space Administration, Huntsville, AL. George C. Marshall Space Flight Center.

Keywords: \*Ignition, \*Laser heating, \*Waspaloy, \*Combustion, \*High pressure oxygen, Carbon dioxide lasers, Nickel alloys, Graphs(Charts), Oxygen supply equipment, Pressurized cabins.

The development of ignition and combustion in pressurized oxygen atmospheres was studied for the nickel-based alloy UNS N07001. Ignition of the alloy was achieved by heating the top surface of a cylindri-cal specimen with a continuous-wave CO2 laser. Two heating procedures were used. In the first, laser power was adjusted to maintain an approximately linear increase in surface temperature. In the second, laser power was periodically increased until autoheating (self-heating) was established. It was found that the alloy would autoheat to combustion from temperatures below the solidus temperature. In addition, the alloy had a tendency to develop combustion zones (hot spots) at high oxygen pressures when the incremental (step) heating test mode was used. Unique points on the temperature-time curves that describe certain events are defined and the temperatures at which these events occur are given for the oxygen pressure range of 1.72 to 13.8 MPa (250 to 2000 psia).

PB91-147280 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Chemical Kinetics Div.

Mechanism of Soot Formation in Acetylene-Oxygen Mixtures.

Final rept.

M. Frenklach, D. W. Clary, W. C. Gardiner, S. E. Stein, and T. Yuan. 1986, 37p

Pub. in Combustion Science and Technology 50, n1-3

p79-115 1986.

Keywords: \*Acetylene, \*Soot, \*Oxygen, \*Reaction kinetics, Computation, Decomposition reactions, Pyrolysis, Chemical reactions, Chemical radicals, Shock tubes, Reprints

A computational study of the chemical kinetic effects of oxygen addition on the process of soot formation

from hot acetylene is reported. The results, which are supported by trends observed in shock-tube experiments, reveal that the reaction pathway to soot identified previously for acetylene pyrolysis remains essentially unchanged in a oxidative environment. The main effects of oxygen are: (1) promotion of fuel decomposition, which slightly alters the initiation route to soot; (2) supplementary rapid production of hydrogen atoms in the initial, small-molecule reactions, which drives the the initial, small-molecule reactions, which drives the concentration of hydrogen above the equilibrium value with respect to H(2) and thus enhances polymeric growth of polycyclic aromatics; (3) oxidation of aromatic radicals by molecular oxygen, which removes them from the polymeric growth. The computational results indicate a crucial need for kinetic studies of high-temperature reactions between molecular oxygen and hydrocarbon radicals. drocarbon radicals.

100.538

PB91-147306 Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Fire Science and Engineering Div.

Radiant Heat Fluxes from 100-200 MW Natural

Gas/Air Diffusion Flames.

Final rept.

J. P. Gore, G. M. Faeth, D. Evans, and D. B.

Pfenning. 1987, 4p
Pub. in Proceedings of Fall Technical Meeting Chemical and Physical Processes in Combustion, San Juan, PR., December 15-17, 1986, p21.1-21.4 1987.

Keywords: \*Diffusion flames, \*Thermal radiation, \*Radiative heat transfer, 'Natural gas, 'Heat flux, Heat transfer, Combustion, Flame propagation, Flames, Flame temperature, Radiant flux density, Reprints.

Extended abstract on the calculation of radiation from 100-200 MW natural gas/air diffusion jet flames.

100 539

PB91-147934 Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Chemical Process Metrology Div.

Velocity and Droplet Size Measurments in a Fuel Spray.

Final rept.

C. Presser, A. K. Gupta, R. J. Santoro, and H. G.

Semerjian. 1986, 11p Sponsored by Department of Energy, Washington, DC. Pub. in Proceedings of AIAA Aerospace Sciences Meeting (24th), Reno, NV., January 6-9, 1986, p1-11.

Keywords: \*Kerosene, \*Flame spraying,
\*Drops(Liquids), \*Particle size distribution, Air flow, Keywords: Mass transfer, Light scattering, Swirling, Velocity, Re-

Experimental results are presented for size, number density and velocity of droplets in a pressure atomized, hollow cone kerosene spray introduced into nonswirling and swirling air flow fields. Laser Doppler velocimetry has been employed to measure the axial, radial and tangential velocity components of the spray droplets, introduced at the exit plane of a moveable-vane swirl-stabilized burner. Spatial distributions of droplet size and number density have been obtained by utilizing an ensemble light scattering technique, based on the measurement of the polarization ratio. Lorenz-Mie calculations of the scattering characteristics of a poly-dispersion of droplets have been carried out to complement the light scattering measurements. High speed cinematography was also used to observe the overall qualitative features of the spray and flame. The results reveal that swirl has a significant influence on the spray jet spread downstream of the nozzle where fuel/air mixing occurs. Swirl modifies both the droplet size and number density, in addition to the expected modification of the velocity distribution. A large number of droplets are captured by the centrally located recirculation region and returned back upstream. These droplets are then transported radially outwards into the surrounding combustion air. The correlation between fuel droplet size and velocity due to its interaction with the swirled combustion air is of major importance toward understanding the phenomenological trends associated with spray flames.

100,540

PB91-148056 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Fire Measurement and Research Signal Detection Efficiency in Multiphoton Ionization Flame Measurements.

Final rept.

K. C. Smyth, and P. J. H. Tjossem. 1990, 8p Pub. in Applied Optics 29, n33 p4891-4898, 20 Nov 90.

Keywords: \*Diffusion flames, Multi-photon processes, Signal detection, Carbon monoxide, Argon, Methane, Fluorescence, Reprints, \*Multiphoton ionization.

Multiphoton ionization is often the most sensitive method available for detecting radical species in flame environments. To make accurate relative concentration measurements, however, the electron (or ion) detection efficiency as a function of flame position must be known. Two methods are presented for determining this quantity in a laminar CH4/air diffusion flame burning at atmospheric pressure. The results show significant variation of the electron detection efficiency in the lean, stoichiometric, and rich flame regions, with the greatest detection sensitivity observed in the high-temperature, primary reaction zones (i.e., near stoichio-metric conditions). Corrections to multiphoton ionization data obtained for H atoms are discussed in terms of determining relative concentration profiles across the methane/air diffusion flame.

100.541

PB91-149013 Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Thermophysics Div.

Laser Diagnostics for Characterization of Fuel Sprays.

Final rept.

C. Presser, A. K. Gupta, R. J. Santoro, and H. G. Semerjian. 1987, 8p

Sponsored by Department of Energy, Washington, DC. Pub. in Proceedings of International Congress on Applications of Lasers and Electro-Optics (5th), ICALEO '86, Arlington, VA., November 10-13, 1986, p160-167 1987

Keywords: \*Fuel sprays, Drop size, Density(Number/volume), Light scattering, Laser applications, Combustion, Reprints, Phase Doppler velocimetry, Deconvelu-

Experimental measurements are presented for a pressure-atomized hollow cone spray introduced into nons-wirling and swirling air flow fields. An ensemble light scattering technique, based on measurement of the polarization ratio, is used to obtain detailed information on mean droplet size and number density in dense regions of the spray. The results reveal that combustion air swirl has a significant influence on the spray structure. Mean droplet size on the spray boundary is found to be larger than that on the centerline for both the nonswirling and swirling cases.

PB91-157180 PC A12/MF A02 California Inst. of Tech., Pasadena. Guggenheim Jet Propulsion Center.

Species Produced in Fires Burning in Two-Layered

and Homogeneous Vitiated Environments.
Rept. for 1 Aug 89-31 Jul 90.
J. H. Morehart, E. E. Zukoski, and T. Kubota. Dec 90, 275p NIST/GCR-90/585

Grant NANB900958

Sponsored by National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Center for Fire Re-

Keywords: \*Combustion products, \*Diffusion flames, \*Stoichiometry, Natural gas, Plumes, Fires, Combustion, Ethylene, Chemical reactions, Air, Pyrolysis.

The chemical species produced in a buoyant, turbulent diffusion flame exposed initially to a supply of fresh air and extending into a reduced-oxygen environment containing products of combustion are investigated. The stably stratified, vitiated region is formed by placing a hood above a burner so that it accumulates the gases of the fire plume, while the direct injection of air into the upper portion of the hood allows conditions to be studied where the stoichiometry of the collected gases is different than that of the plume flow crossing the interface between these two regions. Measure-ments of the composition show that the species produced in the flame depend primarily on the stoichiometry of the gases in the vitiated region, but are independent of the fuel-air ratio of the mass transported across the interface by the plume. Experiments were conducted with natural gas, ethylene, and propylene fuels. For natural gas fires, a weak dependence of species con-

# **COMBUSTION, ENGINES, & PROPELLANTS**

### Combustion & Ignition

centrations on the temperature of the product gas layer was observed over the range 500 to 900K.

PB91-157206 PC A07/MF A01 California Univ., Berkeley. Dept. of Mechanical Engineering.

Fire Propagation in Concurrent Flows.
Final progress rept. 1 Aug 89-31 Jul 90.
A. C. Fernandez-Pello. Dec 90, 133p NIST/GCR-90/ 586

Grant NANB7D0737

See also PB90-151754. Sponsored by National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Center for Fire Research.

Keywords: \*Flame propagation, \*Fire tests, \*Air flow, Flames, Mathematical models, Experimental data, Combustion, Ignition, Burning rate, Turbulent flow, Velocity measurement.

A research program is being conducted to study the mechanisms controlling the spread of fire in turbulent forced gas flows moving in the direction of flame propagation. The research tasks completed during the reporting period include experimental studies of the effect of flow turbulence on the rate of concurrent flame spread, and of mass burning when the combustible material is in a floor configuration. The results of the experiments with thick PMMA sheets show that flow turbulence affects significantly the flame spread and mass burning processes. As the turbulence intensity is increased, the flame spread rate decreases because the flame length sharply decreases, and the mass burning rate increases because the surface heat flux increases. Currently underway is a complementary study with the combustible material placed in a ceiling geometry to observe the effect of buoyancy on the flame spread and mass burning processes. An additional task also completed during the period is a review of the processes of ignition and flame spread of solid combustibles. The review presents a novel approach to the analysis and prediction of both processes based in their close interrelationship.

100,544 PB91-174474 Not available NTIS National Bureau of Standards (NEL), Boulder, CO. Chemical Engineering Science Div.

Ignition Characteristics of Selected SSME Alloys.

J. W. Bransford, P. A. Billiard, J. A. Hurley, and I.

Vasquez. 1986, 21p Contract H43201B

Sponsored by National Aeronautics and Space Administration, Huntsville, AL. George C. Marshall Space

Pub. in Proceedings of NASA Conference on Advanced Earth-to-Orbit Propulsion Technology, Huntsville, AL., May 13-15, 1986, p366-386.

Keywords: \*Heat resistant alloys, \*Metals, \*Combustion, \*Ignition temperature, Laser heating, Differential thermal analysis, Phase transformations, Oxygen supply systems, Hyperbaric oxygenation, Oxides, Re-

Data from the measurement of the surface and interior temperatures of laser heated cylindrical specimens and from Differential Thermal Analysis (DTA) thermograms have shown that the ignition of alloys is a com-plex process. The complexity of the process arises from the numerous complex oxides that are formed during the heating process prior to alloy ignition. The ignition process can involve one or more phase transitions and can also be dependent upon the experimental procedures. The ignition temperature as a function of oxygen pressure has been determined for a series of alloys used in or proposed for use in high pressure oxygen systems. The results for five alloys - UNS N07001, N07718, N07750, S30403, and R30188 - are presented and discussed.

PB91-174797 Not available NTIS National Bureau of Standards (NEL), Gaithersburg,

MD. Center for Fire Research.
Letter to the Editor, Fire Technology, Comments on T.Z. Harmathy Viewpoint, May 1985.

Final rept. D. Gross. 1985, 3p

Pub. in Fire Technology 21, n4 p324-326 Nov 85.

Keywords: \*Heat transfer, \*Absorptivity, \*Inertia, \*Fires, Heat flux, Heat transmission, Transport properties, Thermodynamic properties, Absorption, Reprints.

Comments on Viewpoint by T.Z. Harmathy, Fire Technology, May 1985 (rho) or the square root of K(rho)c-Thermal Inertia or Thermal Absorptivity.

100,546 PB91-175331 Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Fire Safety Technology Div. Surface Flame Spread.

Final rept.

Pub. in SFPE (Society of Fire Protection Engineers)
Handbook of Fire Protection Engineering, Chapter 24, p360-367 1988.

Keywords: \*Flame propagation, \*Fires, Flames, Combustion, Combustible flow, Combustion physics, Liquid fuels, Forest fires, Mathematical models, Burning rate,

The contribution is intended for a proposed handbook currently being organized by a committee of the Society of Fire Protection Engineers. It attempts to address the student or practicing fire protection engineer by its tutorial format. It covers both opposed flow and windaided flame spread over solids in some detail. Approximate formulas are developed using simple assumptions in order to illustrate the role of the relevant physical and chemical variables. The relationship between these approximate formulas and more exact results and data are discussed. Although an extensive review is not presented, an attempt is made to illustrate the extent of knowledge and opportunities for application. Flame spread over liquid fuels and in the forest are briefly discussed.

100,547 PB91-178830 PC A03/MF A01 PB91-178830 PC A037MF A01 National Inst. of Standards and Technology (BFRL), Gaithersburg, MD. FIREDOC Users Manual, 2nd Edition. N. H. Jason. Mar 91, 36p NISTIR-4526 See also PB90-271800.

Keywords: \*Fire research, \*Information dissemination, \*Information retrieval, \*User manuals(Computer programs), Data bases, Bibliographies, US NIST, On line systems, \*FIREDOC systems, \*Fire Research Information Computer (Information Computer Comp mation Services.

FIREDOC is the on-line bibliographic database which reflects the holdings (published reports, articles, books, and audiovisual items) of the Fire Research Information Services (FRIS), at the Building and Fire Research Laboratory, National Institute of Standards and Technology. The manual provides a step-by-step technique for entering and exiting the database via telecommunication lines, as well as a number of techniques for searching the database and processing the results of the searches. The Second Edition incorporates changes from a recent STAR software upgrade, a section of Advanced Techniques and procedures for using FIREDOC with an IBM PC, XT, AT and compatible computers and with a Macintosh computer.

PB91-203794 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Fire Measurement and Research

Div.

Kinetic Properties of the Components of Douglas-Fir and the Heat of Combustion of Their Volatile Pyrolysis Products. Final rept.

W. J. Parker, and S. L. LeVan. 1989, 17p Pub. in Wood and Fiber Science 21, n3 p289-305

Keywords: \*Douglas fir wood, \*Pyrolysis, \*Combustion products, \*Heat of combustion, Cellulose, Lignin, Xylans, Nitrogen, Activation energy, Mass balance, Reprints.

Specimens of the chemical components of Douglas-fir which include cellulose, lignin, mannan, and xylan were pyrolyzed in nitrogen in the temperature range between 290 and 370 C, which is characteristic of the pyrolysis temperature range of wood in a fire environ-ment. From the data the effective activation energy, preexponential factor, and the net heat of combustion of the volatiles were calculated as a function of mass retention fraction of the specimen. The kinetic parameters were used to calculate the mass loss rate of Douglas-fir and a prepared mixture of the components in a pyrolyzer based on their measured temperature history. The calculated mass loss rates were compared with the measured values.

100.549

Not available NTIS PB91-203851 National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Fire Measurement and Research

Wind Effects on Fires.

Final rept.

W. M. Pitts. 1991, 52p

Sponsored by Defense Nuclear Agency, Washington,

Pub. in Progress in Energy and Combustion Science 17. p83-134 1991.

Keywords: \*Fires, \*Urban areas, \*Nuclear explosion effects, Firestorms, Wind(Meteorology), Models, Re-

In the review characteristics of the two types of mass fire--fire storm and conflagration--are discussed. Brief histories of urban mass fire and research efforts on the topic are given. Models which have been developed to predict the initiation, development, spread, and behavior of mass fires following the detonation of a nuclear device in an urban environment are summarized. The current understanding of the fire processes which are believed to control mass fire behavior are reviewed. Particular emphasis is placed on the wind-fire interactions mentioned in the last paragraph. The discussion forms the basis for an analysis of the effectiveness of existing models for mass fire growth and behavior. It is concluded that the understanding of the important physical processes is incomplete and that models for mass fire development and behavior are likely to be subject to large and uncharacterized errors. The possibility of improving our understanding of the underlying physical and chemical processes utilizing reduced-scale experiments is assessed.

100,550

PB91-203869 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Chemical Process Metrology Div. Effect of Atomization Air on Droplet Dynamics of Spray Flames. Final rept.

C. Presser, A. K. Gupta, and H. G. Semerjian. 1988,

Sponsored by Department of Energy, Washington, DC. Pub. in Proceedings of Fall Technical Meeting on Chemical and Physical Processes in Combustion, Clearwater Beach, FL., December 5-7, 1988, p105-1-

Keywords: \*Atomization, \*Sprays, \*Flames, \*Droplets, \*Dynamics, Combustion, Spatial distribution, Aerodynamic characteristics, Flow visualization, Reprints, Atomization air.

Fuel spray combustion is an important part of a wide variety of propulsion and power systems such as furnaces and gas turbine combustors, afterburners, fuelnipection internal combustion engines, liquid rocket engines, etc. Recent studies using air-assist nozzles have shown that the design and fabrication of these nozzles can directly influence spray circumferential uniformity, i.e., the presence of asymmetrical fuel flux profiles in combustors. The practical implications of these fuel flux nonuniformities are that they seriously alter the spray structure, which subsequently affects droplet/air interactions, local fuel/air mixing, overall flame characteristics and combustor performance, and pollutant emission levels. In addition, the effect of aerodynamic factors (i.e., combustion air swirl and atomization air flow rate) on spray characteristics has been investigated. The paper discusses the effect of atomization air on the droplet dynamics of spray flames formed by an air-assist nozzel. Presented are spatial distributions of mean droplet velocity and their probability distributions, which provide quantitative in-formation for examination of the observed spray flame features.

tion, Des Plaines, IL.

PB91-216804 PC A03/MF A01 National Inst. of Standards and Technology (BFRL), Gaithersburg, MD. Interaction of an Isolated Sprinkler Spray and a

Two-Layer Compartment Fire Environment.
L. Y. Cooper. May 91, 49p NISTIR-4587
Sponsored by American Architectural Mfrs. Associa-

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### Combustion & Ignition

Keywords: \*Fire tests, \*Sprinkler systems, Spraying, Mathematical models, Nozzles, Computerized simulation, Water, Combustion, Buildings.

A mathematical model is developed to simulate the interaction of an isolated operating sprinkler and a two-layer fire environments under arbitrary conditions of sprinkler-nozzle elevation, and upper- and lowerlayer thickness and temperature. The sprinkler is characterized by water flow rate, nozzle diameter, and three other device parameters. The model takes ac-count of all effects of the sprinkler spray as it entrains drives downward (by aerodynamic drag on the spray drops), humidifies, and cools (by drop evaporation) gases from both the high temperature upper layer and the relatively cooler lower layer. The model provides a means of predicting the rates of flow of mass, enthalpy, products of combustion, and evaporated water to each of the two layers as a result of sprinkler operation. An algorithm for such predictions is presented in a manner that is suitable for general use in two-layer zone-type compartment fire models. The model is exercised in example calculations which simulate the interaction between the spray of a real sprinkler device and both fire and non-fire environments. The calculations revealed an important generic interaction phenomenon, namely, an abrupt and large change in the growth rate of an upper layer that would accompany an increase in upper layer thickness beyond a critical thickness (for a given upper layer temperature) or an increase in upper layer temperature beyond a critical temperature (for a given upper layer thickness). Exceeding critical values would lead to very large rate of growth of upper layer thickness, a growth that would likely lead to rapid and complete smoke filling of even the largest compartments of fire origin.

100,552 PB91-216838 PC A99/MF E08 National Inst. of Standards and Technology (CSTL), Gaithersburg, MD.

ICLASS-91 Proceedings of the International Con-ference on Liquid Atomization and Spray Systems (5th). Held in Gaithersburg, MD. on July 15-18, 1991.

Special pub. (Final) H. G. Semerjian. Jul 91, 874p NIST/SP-813 Also available from Supt. of Docs. as SN003-003-03086-4.

Keywords: \*Meetings, \*Atomization, \*Sprays, \*Liquids, Atomizers, Diesel engines, Spraying, Atomizing, Fuel systems, Fuel sprays, Metal powder, Combustion, Size determination, Drops(Liquids).

The NIST Special Publication contains the Proceedings of the Fifth International Conference on Liquid Atomization and Spray Systems, sponsored and organized by the Institute for Liquid Atomization and Spray Systems (ILASS-Americas) and the National Institute of Standards and Technology (NIST), held at NIST, in Gaithersburg, Maryland on July 15-18, 1991. One hundred papers were presented at the Conference, including four keynote lectures on Physics of Atomization, Experimental and Theoretical Studies on the Structure of Fuel Sprays in Diesel Engines, Atomization of Liquid Metals for the Manufacture of Metal Powder and for Spray Forming, and Twin Fluid Atomization: Factors In-Spray Forming, and I win Fluid Atomization: Factors Influencing Mean Drop Size. Technical sessions were organized on Evaporation and Mass Transfer in Sprays, Spray Coating, Basic Atomization Processes, Pressure Atomizers, Diesel Sprays, Drop Size Distribution of Sprays, Novel Atomizers, Diagnostics, Atomization of Special Liquids, Spray Combustion, Twin Fluid Atomization, Spray Modeling, Airblast and Electrostatic Atomization, and Airbreathing and Rocket Engines.

PB91-237024 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Fire Measurement and Research

Partial Equilibrium in Laminar Hydrocarbon Diffusion Flames. Final rept.

J. H. Miller, and K. C. Smyth. 1988, 4p Pub. in Chemical Physics Process Combustion, p16/1-

16/4 1988.

Keywords: \*Diffusion flames, \*Hydrogen, \*Oxygen, \*Atoms, Hydroxyl radicals, Hydrocarbons, Equilibrium, Chemical radicals, Reprints, Flame structure, Combus-

Possible methods of estimating H-atom and O-atom concentrations from OH- and major species measure-

ments are discussed. Assumptions of full and partial equilibrium are examined.

PB91-237099 Not available NTIS National Inst. of Standards and Technology (BFRL), Gaithersburg, MD. Fire Measurement and Research Div.

Laser-Induced Fluorescence of CH. in a Laminar CH4/Air Diffusion Flame: Implications for Diagnostic Measurements and Analysis of Chemical Rates. Final rept.

S. Norton, and K. C. Smyth. 1991, 20p Pub. in Combustion Science and Technology 76, p1-

Keywords: \*Methane, \*Diffusion flames, \*Combustion kinetics, Laser applications, Free radicals, Aromatic polycyclic hydrocarbons, Concentration(Composition), Hydrogen atoms, Reprints, \*Laser induced fluores cence, \*Methyl radicals.

Relative CH radical concentration profiles have been measured in a laminar, flowing methane/air diffusion flame using laser-induced fluorescence from the (0,0) band of the A(sup 2)delta--> X(sup 2) pi transition. CH has the narrowest profile of any species yet measured in the flame. The CH peak does not coincide with the position of the OH and temperature maxima, but appears on the fuel-rich side, between the peak concentrations of hydrogen atoms and methyl radicals. If CH fluorescence is detected with a narrow bandpass dielectric filter, rather than using a monochromator, severe interference attributed to fluorescence from polycyclic aromatic hydrocarbons (PAH) is observed. The CH concentration decreases, while PAH fluorescence interference increases rapidly with height above the burner. Implications for CH imaging experiments in turbulent diffusion flames are discussed. The net chemical production/destruction rate of CH is determined as a function of flame position at a height H of 9 mm above the burner. The CH production rate profile is used to derive a relative mole fraction profile for triplet methylene 3CH2. The concentration ratio (3)CH2:max/(CH)max is found to be 13-300, where the major source of uncertainty is the reaction rate of (3)CH2: + H --> CH + H2. Maximum concentrations of the CH, radicals are not well established in the flame. However, if the derived ((3)CH2:)max/(CH.)max ratio is combined with the calculated value of 25 ppm for ((3)CH2:)max from Puri et al. (1987), one estimates that the peak CH mole fraction lies between 0.08 and 2 ppm at H - 9mm.

Not available NTIS PR91-237412 National Bureau of Standards (NEL), Gaithersburg,

MD. Fire Science and Engineering Div.

Experimental Study of the Pyrolysis Rate of a Poly(methyl methacrylate) (PMMA) Wall Panel in a Reduced-Scale Enclosure.

Final rept. K. D. Steckler, and H. E. Mitler. 1988, 4p Pub. in Chem. Phys. Processes Combust., p73/1-73/4 1988

Keywords: \*PMMA, \*Plastics, \*Construction materials, \*Pyrolysis, Combustion chambers, Reaction kinetics, Wallboard, Panels, Fire tests, Flammability, Mathematical models, Comparison, Ventilation, Linings, Reprints.

A series of experiments was conducted to study the pyrolysis rate of a fully-ignited fixed-area wall panel in a reduced-scale enclosure for a wide range of ventilation conditions. The wall panel was PMMA, a non-charring homogeneous material which is amenable to theoretical analysis. Experimental results are compared with theoretical results obtained from a steady-state algebraic model for non-charring, non-melting, homogeneous materials.

PC A11/MF A03 PR92-112432 Michigan State Univ., East Lansing. Dept. of Mechanical Engineering.

Theoretical Investigation of Piloted Ignition of Wood.

L. S. Tzeng, and A. Atreya. Aug 91, 230p NIST/ GCR-91-595 Grant NANB8D0861

Sponsored by National Inst. of Standards and Technology (BFRL), Gaithersburg, MD.

Keywords: \*Wood fuels, \*Combustion, \*Pvrolvsis. Solids, Flame propagation, Gases, Equations, Diffusion flames, Mathematical models, Activation energy, Ignition, Heat transfer, Predictions, Pilot lights.

A theoretical model for piloted ignition of a flame in the gas phase above a vaporizing or pyrolyzing solid has been developed. Using the model it has been found that (1) The postulated simplified governing equations adequately explain the pre-ignition flashes that are often observed experimentally; (2) A rational criterion for positioning the pilot flame exists; (3) The heat losses to the surface play an important role, indicating that the fuel evolution rate by itself is insufficient for predicting the onset of piloted ignition. In the investiga-tion, a numerical integration scheme is developed that accounts for the often vastly different rates between chemical reaction and convection or diffusion processes in the equations of combustion theory. The new numerical scheme is found to be very efficient for the piloted ignition problem, which involves both pre-mixed and diffusion flames. Finally, a numerical model for piloted ignition of wood which includes transient solidphase decomposition has been developed. It has been found that the activation energy for the combustion of the evolved fuel is 49 Kcal/mole.

100,557

PB92-112473 PC A04/MF A01 National Inst. of Standards and Technology (BFRL), Gaithersburg, MD.

Data for Fire Hazard Assessment of Selected Non-Halogenated and Halogenated Fire Retardants; Report of Test FR 3983.

R. H. Harris, V. Babrauskas, B. C. Levin, and M.

Paabo. Oct 91, 56p NISTIR-4649
Sponsored by Huber (J.M.) Corp., Norcross, GA. Solem Div., and Aluminum Co. of America, Alcoa Center, PA. Alcoa Technical Center.

Keywords: \*Fire resistant materials, \*Plastics, \*Fire hazards, \*Flammability testing, Halogens, Additives, Comparison, Toxicity, Calorimetry, Combustion products ucts, Thermal degradation, Hydrogen chloride, Hydrogen bromide, Smoking, Ignition, Gases, Cone calori-

Five plastic materials, with and without fire retardants, were studied to compare the fire hazards of non-halogenated fire retardant additives with halogenated flame retardants. The plastic materials were identified by the sponsors as unsaturated polyesters, thermoplastic high density, low density and cross-linked low density polyethylenes, polypropylene, flexible and rigid poly(vinyl chlorides), and cross-linked and thermoplastic ethylene-vinyl acetate copolymers. The non-halogenated fire retardants tested were aluminum hydroxide (Al(OH)3), also known as alumina trihydrate (ATH), sodium alumino-carbonate, and magnesium hydroxide. The halogenated flame retardants were chlorine or bromine/antimony oxides. The plastics were studied using the Cone Calorimeter and the cup furnace smoke\_toxicity\_method (high\_density\_polyethylene only). The Cone Calorimeter provided data on mass consumed, time to ignition, peak rate and peak time of heat release, total heat released, effective heat of combustion, average yields of CO, CO2, HCl, and HBr, and average smoke obscuration. The concentrations of toxic gases generated in the cup furnace smoke toxicity method were used to predict the toxic potency of the mixed thermal decomposition products. The data from the Cone Calorimeter indicate that the non-halogenated fire retardants were, in most of the tested plastic formulations, more effective than the halogenated flame retardants in increasing the time to ignition. The non-halogenated fire retardants were also more effective in reducing the mass consumed, peak rate of heat release, total heat released, and effective heat of combustion, and in reducing the amount of smoke produced. The use of halogenated flame retardants increased smoke production and CO yields and, additionally, produced the known acid gases and toxic irritants, HCl and HBr, in measureable quantities.

100 558

PB92-117191 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Fire Measurement and Research

Large-Scale Turbulent Structures and the Stabilization of Lifted Turbulent Jet Diffusion Flames. Final rept.

W. M. Pitts. 1990, 8p

Pub. in Proceedings of International Symposium on Combustion/The Combustion Institute (23rd), Orleans, France, July 22-27, 1990, p661-668.

# **COMBUSTION, ENGINES, & PROPELLANTS**

### Combustion & Ignition

Keywords: \*Diffusion flames, \*Vortices, \*Jet flow, Turbulence, Rayleigh scattering, Turbulent flow, Light scattering, Velocity measurement, Flame photometry, Hot wire anemometers, Combustion stability, Reprints.

The physical mechanisms responsible for the stabilization of lifted axisymmetric turbulent jet diffusion flames remain uncharacterized. Flame stabilization has been shown to take place at radial locations in the corresponding isothermal jets where the flow has an intermittent character. Recently developed flow diagnostics capable of simultaneous multi-point concentration and velocity measurements are used to investigate the large-scale turbulent structures in the intermittent region of an isothermal jet of propane. The findings, in conjunction with earlier literature results, show that large-scale structures form as the result of organized turbulent motion during which strong outward ejections of fluid form central regions of the jet flow into the ambient surroundings. Once formed, the large-scale structures are convected downstream for long distances. The downstream edges of the structures are regions of significantly higher concentration gradients and shear than regions further upstream. Occasionally, the jet fluid loses its turbulent energy and is no longer transported by the flow. The fluid can be reentrained by the passage of later large-scale structures. It is concluded that the processes responsible for flame stabilization must occur in these large-scale turbulent structures.

100 559 PB92-117365 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Fire Measurement and Research

Relative H-Atom and O-Atom Concentration Measurement in a Laminar, Methane/Air Diffusion Flame.

Final rept.

K. C. Smyth, and P. J. H. Tjossem. 1990, 9p Pub. in Proceedings of Symposium on Combustion/ The Combustion Institute (23rd), France, July 22-27, 1990, p1829-1837.

\*lonization, Keywords: \*Diffusion \*Concentration(Composition), \*Fluorescence, \*Laser applications, Quantitative analysis, Chemical analysis, Electrophotometry, Laser beams, Methane, Hydrogen, Flame photometry, Laser spectroscopy, Laminar flow, Oxygen, Reprints.

Relative H-atom and O-atom concentration profiles have been measured in a laminar, co-flowing methane/air diffusion flame burning at atmospheric pressure. Multiphoton ionization (2 + 1 process at 243 nm) has been used to detect H atoms, while laser-induced fluorescence at 845 nm excited by two-photon absorption at 226 nm was employed to observe O atoms. In both cases it was found that low photon intensities were required in order to avoid the photolytic producwere required in order to avoid the photolytic produc-tion of the species of interest. Doppler-free measure-ments were carried out using a retroreflected-beam geometry in order to provide sufficient signal levels. Under these experimental conditions it is necessary to correct the raw profile data for variations in collisional quenching and electron detection sensitivity as a function of flame position. Establishing absolute radical concentrations is discussed in terms of partial equilibrium considerations and detailed flame structure calculations.

### **Fuel & Propellant Tanks**

100,560 PB91-175570 Not available NTIS National Inst. of Standards and Technology, Boulder, CO. Chemical Engineering Science Div.

Reusable Cryogenic Foam Insulation for Advanced Aerospace Vehicles.

Final rept. P. S. McAuliffe, A. H. Taylor, L. L. Sparks, and W. P.

Dube. 1991, 12p Pub. in Proceedings of AIAA Aerospace Sciences Meeting (29th), Reno, NV., January 7-10, 1991, p1-12.

Keywords: \*Propellant tanks, \*Thermal insulation, \*Cryogenic fluid storage, Cryogenic rocket propellants, Rocket propellants, Storage tanks, Fuel tanks, Thermal conductivity, Foams, Aerospace vehicles, Reprints.

Future high-speed aircraft and aerospace vehicles using cryogenic propellants will require an advanced reusable insulation system for the propellant tank structure. The cryogenic insulation system must be lightweight, structurally and thermally efficient, and capable of multiple reuse without cracking or degraded performance. The paper presents recent progress in the development of a reusable cryogenic foam insulation system having a maximum service temperature of 400 F. The system consists of pre-shaped, pre-cut blocks of rigid polymethacrylimide foam insulation, wrapped with a high-temperature. Kapton and aluminations are supported by the control of the num foil vapor barrier which is adhesively bonded to the propellant tank well.

### **Reciprocation & Rotating Combustion Engines**

100.561 PB91-189498 Not available NTIS National Inst. of Standards and Technology (IMSE), Gaithersburg, MD. Ceramics Div. Ceramic Wear Maps.

S. M. Hsu, D. S. Lim, and R. G. Munro. 1988, 10p Pub. in Proceedings of the International Symposium on Ceramic Materials and Components for Engines (3rd), Las Vegas, NV., November 27-30, 1988, p1236-1245.

Keywords: \*Wear, \*Ceramics, \*Graphic methods, \*Tribology, \*Heat engines, Friction, Mapping, Tests, Methodology, Reprints.

Friction and wear characteristics of ceramics are crucial properties for their successful application to new engine designs. Tests for friction and wear performance usually are based on empirical field trials. These tests are very expensive. Laboratory measurements of tribological properties would be much less expensive. However, laboratory tests are specific to a particular wear tester and the specific operating conditions. Translation of laboratory results to industrial application and design is often difficult and fraught with uncertainty. The paper describes a new systematic effort to measure and represent the wear characteristics of ceramics in a uniform and unified methodology. For any material, the methodology leads to a set of wear maps which collectively provide a comprehensive representation of the wear properties of the materials. The maps provide critical guidance to design engineers for materials selection.

# COMMUNICATION

### Common Carrier & Satellite

FIPS PUB 159 PC **E07** National Inst. of Standards and Technology (CSL), Gaithersburg, MD. Detail Specification for 62.5-mum Core Diameter/ 125-mum Cladding Diameter Class la Multimode, Graded-Index Optical Waveguide Fibers. Graded-Index Optical Waveguide Fibers.
Federal information processing standards (Final).
S. M. Radack, and A. G. Hanson. 27 Dec 90, 24p
Also pub. as American National Standards Inst., New
York rept. no. ANSI/EIA/TIA-492AAAA-1989. Prepared in cooperation with American National Standards Inst., New York, and National Communications
System, Arlington, VA.
Three ring wind binder also available: North American

Three ring vinyl binder also available: North American

Continent price \$7.00; all others write for quote.

Keywords: \*Standards, \*Optical waveguides, \*Glass fibers, \*Telecommunications, \*Data processing systems, Cladding, Cores, Acceptability, Industries, Protective coatings, Performance tests, Measurement, Attenuation coefficients, Bandwidth, Length, Federal Information Processing Standards.

The standard, by adoption of American National Standard/EIA/TIA-492AAAA-1989, defines the opti-

cal, geometrical, environmental, and mechanical speccal, geometrical, environmental, and mechanical specifications for glass (EIA/TIA-458-A-1984 Class Ia) multimode optical waveguide fibers. Minimum acceptable values for all characteristics are given, and applicable industry standards for their measurement are referenced. The standard supersedes former draft Federal Standard (FED-STD) 1070 in its entirety.

100.563

PB91-134825 Not available NTIS National Inst. of Standards and Technology (NCSL), Gaithersburg, MD. Systems and Network Architecture

Performance of OSI Transport over ACCUNET and IBERPAC.

Final rept.

E. Vazquez, R. Colella, J. Vinyes, J. Fox, and J.

Berrocal. 1988, 10p Sponsored by Universidad Politecnica de Madrid (Spain). Escuela Tecnica Superior de Ingenieros de Telecomunicacion.

Pub. in Proceedings of Annual Joint Conference IEEE (Institute of Electrical and Electronics Engineers) Computer and Communications Societies - IEEE INFO-COM (7th), New Orleans, LA., March 27-31, 1988,

Keywords: \*Computer networks, Simulation, Specifications, Reprints, \*Computer communications, \*Protocols, Throughput.

The paper presents the results of a research project intended to assess the effect of several transport mechanisms on throughput observed between two transport users communicating over concatenated X.25 networks. Two main areas of effort are covered. First, the protocol design and development process is addressed, including the formal specification of class 4 transport and the tools used to support protocol implementation and testing. The main advantages of ESTELLE, the formal specification language used, and the development method are outlined. The second area covered is a set of simulated and live experiments investigating transport performance over X.25 networks. The transport mechanisms of potential interest (splitting, concaternation and acknowledgement with-holding) are described and the main simulation results are presented. Finally, the simulation results are validated with live experiments over two concatenated X.25 networks. As indicated in the conclusion, use of the three mechanisms considered in the paper result in significant transport user throughput improvements.

100,564

PB91-148734 Not available NTIS National Inst. of Standards and Technology (NEL), Boulder, CO. Electromagnetic Fields Div. Quasi-Static Analysis of a Two-Wire Transmission

Line Located at an Interface.

Final rept.
D. A. Hill. 1990, 6p
Pub. in Radio Science 25, n4 p435-440 Jul/Aug 90.

Keywords: \*Transmission lines, Characteristic impedance, Permeability, Permittivity, Interfaces, Reprints.

Simple quasi-static expressions have been derived for the propagation constant, the characteristic impedance, and the field distribution of a two-wire transmission line located at the air-Earth interface. Both the complex permittivity and the complex permeability of the Earth are allowed to differ from the free-space values, and a numerical solution of the mode equation shows that quasi-static approximation is valid when the wire separation is much less than a free-space wavelength. The quasi-static approximation can be used to determine both the complex permittivity and the complex permeability of the Earth from measurements of the propagation constant and the characteristic impedance of the transmission line.

100,565

PB91-158584 Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Building Equipment Div.
Toward Modular Semantic Application Layer Pro-

tocols (MS-ALPs): Communication between Heterogeneous Information Systems Using Artificial Intelligence (AI) Programming Techniques. Final rept.

W. F. Danner. 1986, 10p

Pub. in Proceedings of Annual Technical Symposium (25th) Distributed Information Systems: Emerging

# Common Carrier & Satellite

Uses and Technology, Gaithersburg, MD., June 12, 1986, p63-72.

Keywords: \*Computer communications, \*Protocols, 'Artificial intelligence, Information systems, Computer aided design, Data base management systems, Distributed computer systems, Computer programming, Knowledge representation, LISP programming language, Reprints, Object-oriented programming.

A communication capability between incompatible information systems is presented. Formats for Modular Semantic Application Layer Protocols (MS-ALPs) are described. A Meta-Information (MI) Format supports the exchange of knowledge necessary for each system to understand the other. Subsequently an Information (I) Format provides for the exchange of information in the context of that knowledge while maintaining system semantics. The MS-ALP Formats make use of two artificial intelligence (AI) programming techniques: frame-based knowledge representation; and object-oriented programming capabilities as an integral part of the frame-based representation. These self-descriptive' formats provide for a virtual extension of an information management system (IMS) which does not require a detailed understanding of IMS operations for access to information. An implementation is described which operates within LISP programming environments. However, the concepts developed during the course of this research are believed to have wider applicability.

100.566 Not available NTIS PB91-175018 Mational Bureau of Standards (ICST), Gaithersburg, MD. Systems and Network Architecture Div.

Application of Formal Description Techniques to

the Specification of Distributed Test Systems.

R. J. Linn, and J. P. Favreau, 1988, 14p Pub. in Proceedings of IEEE INFOCOM Conference on Computer Communications, New Orleans, LA., March 27-31, 1988, p96-109.

Keywords: \*Distributed processing, \*Tests, \*Electronic mail, Specifications, Protocols, Distributed computer systems, Translators, Computer networks, Computer communications, Reprints, Department of Defense, OSI(Open Systems Interconnection).

As part of a planned transition by the Department of Defense (DoD) from military standard to Open Systems Interconnection (OSI) protocols, the National Bureau of Standards (NBS) is implementing and testing two application-layer gateways. NBS is applying description techniques developed within the International Organization for Standardization (ISO) and the Consultative Committee for International Telephone and Telegraph (CCITT) to the specification of distributed test systems for the gateways between OSI and DoD networks. Translators, developed at NBS, for Estelle and ASN.I aid in automating the implementation of the test systems. An overview of the test system for an electronic mail gateway and the methods employed to realize it are presented. Measures of productivity of the methods employed are also presented.

100.567 PB91-187682

(Order as PB91-187617, PC A06/MF A01) National Inst. of Standards and Technology, Boulder,

Limited International Intercomparison of Responsivity Scales at Fiber Optic Wavelengths.

sivity Scales at Fiber Optic Wavelengths.

R. L. Gallawa, J. L. Gardner, D. H. Nettleton, K. D.

Stock, T. H. Ward, and X. Li. 1991, 6p

Prepared in cooperation with National Measurement

Lab., Lindfield (Australia), National Physical Lab., Teddington (England), and Physikalisch-Technische Bundesanstalt, Brunswick (Germany, F.R.).

Included in Jnl. of Research of the National Institute of

Standards and Technology, v96 n2 p225-245 Mar/Apr

Keywords: \*Optical communication, Near infrared radiation, Ge semiconductor detectors, Interlaboratory comparisons, Optical detectors, Optical fibers, Fiber optics, Standards, Optical power, Intercomparison.

The authors report here on a recent limited international intercomparison of responsivity scales at wavelengths of interest to the optical communications community. Participants in the comparison were the national laboratories in the United States, the United Kingdom, Germany, and Australia. The wavelengths tested were 1300 and 1550 nm. Data taken at 850 nm are only briefly discussed. The disagreement between the national laboratories' responsivity scale is comfortably within the uncertainty claimed by each laboratory.

100,568 PB91-187724 PC A03/MF A01 National Inst. of Standards and Technology (CSL),

Validation of an OSI Transport Class 4 Simulator. O. Kim, S. Heatley, and B. Bishop. May 91, 36p NISTIR-4530

Keywords: \*Computer communications, \*Computer networks, \*Protocols, Scheduling, Algorithms, Simulation, Models, Computer systems hardware, Computer software, OSI transport.

Most work on scheduling in communications protocols has considered only the MAC layer. Token bus, token ring, and FDDI all have priority mechanisms. But mechanisms. anisms for scheduling must be extended into the upper OSI layers to be effective. The National Institute of Standards and Technology (NIST) has chosen to study possible scheduling mechanisms for Transport Class 4 by first developing a detailed Transport Class 4 simulator. The discrete event simulator is written in Simscript II.5 and simulates the Intel iNA960 implementation of Transport Class 4 running on a 186/51 front-end board with a 286/10 host. In the paper, the model is described, the processing times which serve as inputs into the model are specified and the validation experiments are documented.

PB91-187831 PC A05/MF A01 National Inst. of Standards and Technology (CSL), Gaithersburg, MD. Issues in Transparent File Access.

Special pub. (Final). K. Olsen, and J. Barkley. Apr 91, 90p NIST/SP-500/

Also available from Supt. of Docs. as SN003-003-03079-1.

Keywords: \*Communication networks, \*File management systems, \*Access methods, Operating ment systems, \*Access methods, Operating systems(Computers), Standards, UNIX(Operating system), Semantics, File structures, Access control, Applications programs(Computers), Protocols, Interfaces, Remote systems, Computer programs, NES(Network File System), TFA(Transparent File Access), POSIX.

For a computer system attached to a network, the network provides connectivity to many other systems whose file systems may be very different from the local file system. However, there is no standard way for an application to 'transparently' access files on several file systems whose access characteristics may differ from the access characteristics of the local file system. Transparent file access means that remote files are accessed as though they were local. The Institute of Electrical and Electronics Engineers (IEEE) 1003.8 Transparent File Access (TFA) Working Group of the POSIX Standards Committee (IEEE P1003) has under-POSIX Standards Committee (IEEE F 1003) has directaken the development of an application programming interface specification based on the IEEE 1003.1-1990 Standard. The objective of IEEE 1003.8 is to permit access to the widest possible range of file systems which can resemble the file system of IEEE 1003.1-1990. The report presents the major issues and prob-lems whose resolution form the basis of the IEEE 1003.8 TFA Standard. Some issues are illustrated with examples and demonstrations using the Network File System (NFS), the most widely used implementation for accessing remote files on a network.

Not available NTIS PB91-203091 National Inst. of Standards and Technology (NEL), Boulder, CO. Electromagnetic Technology Div.
Frequency Stabilization of an Erbium-Doped Fiber
Laser: A Potential Wavelength Standard for Optical Communications.

Car Communications:
Final rept.
S. L. Gilbert. 1991, 1p
Pub. in Proceedings of Optical Fiber Communication
Conference, San Diego, CA., February 18-22, 1991,

Keywords: \*Optical communication, Near infrared radiation, Infrared lasers, Tunable lasers, Frequency standards, Frequency stability, Acetylene, Reprints, \*Erbium lasers, Fiber lasers, Wavelength standards.

A single frequency, = or < 1.6 MHz linewidth, tunable Er(+)-doped fiber laser has been constructed. Stabili-

zation to an absorption line of acetylene near 1.53 micrometers reduced the laser frequency noise to less than 500 kHz rms.

PB91-216622 PC A03/MF A01 National Inst. of Standards and Technology (CSL), Gaithersburg, MD.
Electronic Data Interchange in Message Handling

P. Markovitz. Jun 91, 39p NISTIR-4608 Sponsored by Internal Revenue Service, Washington,

Keywords: \*Message processing, \*Electronic mail, Data transmission, Standardization, Computer communications, Protocols, Data structures, Data processing security, Models, Dictionaries, EDI(Electronic Data Interchange), MHS(Message Handling System), IPMS(Interpersonal Messaging Service).

Electronic Data Interchange (EDI) identifies a family of standards used for the electronic transmission of business oriented data (e.g., invoices and purchase orders). EDI standards specify data formats, but are designed independent of a communications protocol. In June, 1990, the Consultative Committee on International Telephony and Telegraphy (CCITT) drafted two Recommendations (F.435:EDI Messaging Service, X.435: EDI Messaging System) which define a standardized service and protocol for transmitting EDI data via the Message Handling System (MHS). Using the MHS, EDI data can be transferred between compatible EDI applications implemented on heterogeneous comstandards used for the electronic transmission of busi-EDI applications implemented on heterogeneous computer systems. The paper introduces the MHS, the carrier service for EDI data; and the Interpersonal Messaging Service, the only MHS application currently standardized and the model for the EDI Messaging Service. Following the introductory material is a detailed review of the EDI Messaging draft Recommendations. The transmission of EDI data via the MHS is described as well as the relationships between EDI Messaging and directory, security, and physical delivery services. Three appendices are also included in the paper. Appendix A contains a list of abbreviations. Appendix B provides a glossary of MHS terms, and Appendix C briefly describes EDI messaging elements of

PB92-102201 PC A05/MF A01 National Inst. of Standards and Technology (NCSL), Gaithersburg, MD. Advanced Systems Div. ISDN Conformance Testing: Layer 1. Physical Layer. Part 1. Basic Rate S/T Interface, User Side.

Special pub. (Final). S. A. Wakid, and K. M. Roberts. Sep 91, 91p NIST/

Also available from Supt. of Docs. as SN003-003-

Keywords: Telecommunication, Test methods, Interfaces, Communication networks, Communications management, \*Integrated Services Digital Network, Test specifications, Conformance tests.

The American National Standard for Telecommunications T1.605-1989 specifies the Layer 1 requirements to provide for satisfactory transmission between a Terminal Equipment (TE) and Network Termination (NT). It describes both the physical interface and the electrical characteristics of the signals appearing at the S and T reference points. Equipment designed to operate on the Integrated Services Digital Network (ISDN) Basic Rate S or T interface must conform with this set of requirements. The document describes a set of test specifications which test conformance of TEs and NTs to the ISDN Physical Layer at the S/T reference point, as defined in ANS T1.605-1989. These tests were developed and approved by members of North American ISDN Users' Forum (NIU-Forum).

100.573

PC A08/MF A02 PB92-102219 National Inst. of Standards and Technology (CSL), Gaithersburg, MD. Advanced Systems Div. North American ISDN Users' Forum Agreements on Integrated Services Digital Network.

Special pub. (Final). A. Wakid, and K. M. Roberts, Sep 91, 152p NIST/

SP-500/195

Also available from Supt. of Docs. as SN003-003-03110-1. See also PB91-171967, PB91-197004, PB92-112200 and PB92-102201.

### COMMUNICATION

### Common Carrier & Satellite

Keywords: \*Standards, Communication networks, Computer networks, Computer software, Specifications, User needs, Tests, \*ISDN(Integrated Services Digital Network), Basic rate interface, Primary rate interface.

The document compiles the existing North American ISDN Users' Forum (NIU-Forum) agreements for an Integrated Services Digital Network (ISDN) developed and approved in the NIU-Forum as of November 1990. These agreements cover: Layer 1 Basic Rate Interface (BRI) at the U, and S/T reference points; Layer 1 Primary Rate Interface (PRI) at the U reference point; Layer 2 BRI and PRI; Layer 3 BRI Basic Call Control for Class I equipment; Layer 3 PRI Basic Call Control for Class II equipment; and Generic Control procedures for Class I BRI Supplementary Services. In addition, the document references the Conformance tests which have been completed by the NIU-Forum. These include: Layer 1 BRI S/T interface; and Layer 2 BRI Link Access Procedure, D-channel (LAPD). Finally, the document contains the Application Profile for four of the Incoming Call Management applications which have been submitted to the NIU-Forum.

### Graphics

100,574

PB91-187773 PC A03/MF A01
National Inst. of Standards and Technology (NCTL),
Gaithershurg MD Office Systems Ferriage Gaithersburg, MD. Office Systems Engineering Group.
Government Document Processing Requirements Report. R. F. Sies. Apr 91, 16p NISTIR-4560

Keywords: \*Standards, Documents, User needs, \*Electronic publishing, Electronic Information Ex-\*Electronic publishing, Electronic Information Exchange Standards, ODA(Office Document Architecture), SGML(Standard Generalized Markup Language), SPDL(Standard Page Description Language), ODL(Office Document Language).

The report describes several activities of the Office Systems Engineering Group in the area of electronic publishing standards. It gives an account of the July 30, 1990 workshop on Electronic Information Exchange Standards Used in Document Processing Applications and the list of User Requirements that came out of that workshop. The report also talks about other efforts the Office Systems Engineering Group has made to help bring about the harmonization of electronic publishing standards.

### Policies, Regulations, & Studies

100.575

N91-25760/0

(Order as N91-25755/0, PC A99/MF A04) National Inst. of Standards and Technology (NML), Boulder, CO. Time and Frequency Div.

Boulder, C.O. Time and Frequency Div. Trapped-lon Frequency Standards.
D. J. Wineland, W. M. Itano, J. C. Bergquist, J. J. Bollinger, and D. J. Heinzen. May 90, 8p
Pub. in Proceedings of Annual Precise Time and Time
Interval (PTTI) Applications and Planning Meeting
(22nd) p53-60 (See N91-25755 17-70). Sponsored by
AFOSR and Onr.

Keywords: Atoms, \*Frequency standards, lons, \*Trapped particles, Clocks, Microwaves, Optical equipment, Radio frequencies, Time measurement.

Frequency standards based on stored atomic ions are briefly reviewed. Specific examples are chosen to illustrate what is currently possible. Both rf/microwave and optical devices are discussed. The present limitations to existing experiments and possibilities for future improvement are outlined.

100,576

N91-25766/7

(Order as N91-25755/0, PC A99/MF A04) National Inst. of Standards and Technology, Boulder, CO

GPS Time Transfer with Implementation of Selec-

tive Availability.

D. W. Allan, M. P. Granveaud, W. J. Klepczynski, and W. W. Lewandowski. May 90, 11p

Pub. in Proceedings of Annual Precise Time and Time

Interval (PTTI) Applications and Planning Meeting (22nd) p145-155.

Keywords: \*Global positioning system, \*Metrology, Navigation satellites, \*Time measurement, Atomic clocks, Navigation, Observatories.

The international community of time metrology is facing a major challenge with the Selective Availability (SA) degradation of GPS satellite signals. At present there are 6 Block 1 satellites and 8 Block 2 satellites operating. According to the policy of the U.S. Department of Defence the Block 1 satellite signals will not be degraded, but these satellites are old with a finite life. The Block 2 satellites, which have all been launched since 1988, were subject to Selective Availradiity from March 25, 1990. The effect of Selective Availability from March 25, 1990. The effect of SA should be to limit precision to about 100 meters for navigation and 167 ns for timing. A study was conducted in order to understand the nature of the actual introduced degradation, and to elaborate the means of removing the effects of this degradation on time transfer. This study concerns the time extraction from GPS satellites at NIST, USNO and Paris Observatory, and the comparison of atomic clocks between these laboratories by common view approach. The results show that when using the data taken over several days the time extraction can be achieved with uncertainty of a few tens of nanoseconds, while strict common-view has removed entirely the effects of SA during the periods under

100,577 PB91-134593 Not available NTIS National Bureau of Standards (NML), Boulder, CO. Time and Frequency Div.
Israel's New Synchronized Time Scale, UTC(INPL).

D. W. Allan. 1988, 5p Pub. in Proceedings of Annual Symposium on Frequency Control 1988 (42nd), Baltimore, MD., June 1-3, 1988, p485-489.

Keywords: \*Time measurement, Cesium frequency standards, Frequency stability, Synchronism, Israel, Reprints, Software clocks.

The National Physical Laboratory of Israel (INPL) together with Time and Frequency Limited (TFL) and NBS is building a software clock to be used as the Israeli national time base, UTC(INPL). The software clock is based on several commercial Cs clocks (HP and TFL) whose outputs are routed sequentially through a TFL programmed switch into a time interval counter. The page presents the principles of concept. counter. The paper presents the principles of generating the software clock, its performance and the method to compare it to UTC and UTC(NBS). The paper also presents the optimization procedures for synchronizing and syntonizing UTC(INPL) with UTC as a coordinated time scale.

100,578 PB91-162388 Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Time and Frequency Div.

Calculated from the Frequency Domain: An

Final rept. F. L. Walls, J. Gary, A. O'Gallagher, L. Sweet, and R. Sweet. 1990, 8p

Pub. in Proceedings of the European Frequency and Time Forum (4th), Neuchatel, Switzerland, March 13-15, 1990, p197-204.

Keywords: \*Frequency stability, Time domain, Reprints, Allan variance, Phase noise.

The authors investigate the dependence of the fractional frequency stability measures and mode on the parameter for common power-law noise types. The authors have implemented the calculations using numerical techniques which make it possible to perform the calculations for virtually any value of the parameter for common power-law noise types and a wide variety of high-frequency filters.

100,579 PB91-192989 PC A06/MF A02 National Inst. of Standards and Technology, Gaithersburg, MD. Office of Standards Services.

Conformity Assessment Workshop on Electromagnetic Compatibility.
B. G. Simson. Jun 91, 111p NISTIR-4611
See also PB91-192997. Sponsored by American Society of Mechanical Engineers, Washington, DC., and American Council of Independent Labs., Washington,

Keywords: \*Electromagnetic compatibility, \*Meetings, Government policies, Recommendations, Competition, European Economic Community, Conformity as-

On April 4, 1991, the National Institute of Standards and Technology (NIST) cosponsored a conformity assessment workshop on electromagnetic compatibility (EMC) with the American Council of Independent Laboratories (ACIL) and the American Electronics Association (AEA). The purpose of the workshop, which focused on information technology equipment (ITE), was to explore how the U.S. Government can assist EMC laboratories in gaining acceptance of their test results in such other markets as the European Community (EC). The following consensus recommendations were reached by the private sector panelists: (1) establishing an EMC advisory committee; (2) harmonizing the National Voluntary Laboratory Accreditation Program (NVLAP) and Federal Communications Commission (FCC) programs; (3) negotiating an agreement with the EC to permit establishing notified bodies in the United States; (4) establishing a formal U.S. Government role in accrediting conformity assessment programs; and (5) establishing a proactive role for NIST in disseminating information in to affected interests in the EMC

100.580 PB91-200790 Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Time and Frequency Div.

New Inexpensive Frequency Calibration Service

from NIST.

D. W. Allan, D. D. Davis, J. Levine, M. A. Weiss, and N. Hironaka. 1990, 10p Pub. in Proceedings of Annual Symposium on Frequency Ccontrol (44th), Baltimore, MD., May 23-25, 1990, p107-116.

Keywords: Frequency stability, Accuracy, Reprints, \*Frequency calibration, Automated computer time system, ACTS system, US NIST.

A new inexpensive frequency calibration service from NIST is now available. The service takes advantage of the operation of the NIST Automated Computer Time System (ACTS), which was begun in 1988. Software to access the service from several types of computers was released at the same time. Time and frequency dissemination by the modest-accuracy service depends on the reciprocity of the telephone system. The round-trip delay is measured by the NIST equipment. round-trip delay is measured by the NIST equipment. The advance of an on-time marker is adjusted so as to arrive at the user's site on time. A frequency calibration method taking advantage of the service has been designed and preliminary tests conducted. A computer is not required to access the service. All that is required is a telephone modem, a simple peripheral circuit to generate an on time marker and standard time and frequency measurement and data processing equipment.

100,581 PB91-200808 Not available NTIS
National Inst. of Standards and Technology (NML),
Boulder, CO. Time and Frequency Div.
Rubidium Frequency Standard and a GPS Receiver: A Remotely Steered Clock System with Good
Short-Term and Long-Term Stability.
Final rept.

D. W. Allan, and J. Levine, 1990, 10p Pub. in Proceedings of Annual Symposium on Frequency Control, Baltimore, MD., May 23-25, 1990,

Keywords: \*Rubidium frequency standards, \*Global positioning system, \*Frequency stability, Cesium frequency standards, Frequency synchronization, Reprints, Time transfer.

The short-term stability of a rubidium gas-cell frequency standard is usually better than that of commercial cesium-beam frequency standards. Cesium almost always has better stability in the long-term because cesium has less sensitivity to environmental perturba-tions. For example, cesium has little or no frequency

# Policies, Regulations, & Studies

drift, whereas rubidium usually does. Improving a clock's environment invariably improves the long-term performance, especially in the case of rubidium. Satellite time transfer shows a day-to-day stability of about a nanosecond. If a rubidium standard, in a good environment with the above performance in the short-term, were married to a satellite time-transfer system, then the combined performance of the system could have better short-term and better long-term stability than a stand-alone, free-running, commercial cesium stand-ard. The authors have taken some data to test the idea. The conclusions confirm the hypothesis. The authors have also replaced the rubidium oscillator with a quartz oscillator and with a high-performance commercial cesium standard. In both cases the system had significantly improved long-term stability over what otherwise would be obtainable from either oscillator by itself.

100.582 PB91-202937 Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Time and Frequency Div. Frequency and Time Stability of GPS and GLON-ASS Clocks.

Final rept.

P. Daly, I. D. Kitching, D. W. Allan, and T. K. Peppler. 1990, 13p Pub. in Proceedings of Annual Symposium on Frequency Control (44th), Baltimore, MD., May 23-25, 1990, p127-139.

Keywords: \*Global positioning system, \*Frequency stability, Frequency standards, Time standards, Atomic clocks, Comparison, Reprints, \*GLONASS system.

The frequency stability and reliability of the clocks are critical to the success of the GPS and GLONASS programs. The authors show some of the similarities and differences between the clocks involved in these two systems. On-board clocks and the stability of the master control clocks for these systems are analyzed. The authors discuss the attributes of these two systems as time and frequency references. Their relationship to UTC will also be illustrated. More data over a longer period of time was available for the authors from GPS than from GLONASS. Even so it is obvious that both systems have matured. Though the GLON-ASS system was developed later, its overall clock performance has improved more rapidly. Some of the more recent GLONASS clock performance is at about the same level as that of the GPS clocks. The analysis has yielded some very interesting contrasts, comparisons, and changes in these systems that should be of great interest for time and frequency users, as well as for clock vendors and receiver vendors.

100,583 PB91-203174 Not available NTIS National Bureau of Standards (NML), Gaithersburg,

Advances in Science, Emerging Technologies and Global Competition: Opportunities and Challenge. Final rept.

H. Hellwig. 1988, 9p Pub. in Proceedings European Frequency and Time Forum (2nd), Neuchatel, Switzerland, March 16-18, 1988, p13-21 1988.

Keywords: \*Frequency standards, \*Time standards, Competition, Technology, Oscillators, Clocks, Reprints.

For the remainder of the century, the time and frequency community is faced with significant new opportunities and challenges. The roots of current time and frequency technology date back half a century; scientific advances have been largely evolutionary and have gradually expanded the boundaries of these known foundations. In stark contrast to this, the technological world is undergoing nearly revolutionary changes which are driven by 3 interrelated forces: Global Competition, Emerging Technologies and Advances in Science. In the following, specific examples of these three areas are described as they relate to time and frequency. The opportunities which can be derived from emerging technologies and scientific advances are quite large, but seemingly require more efficient methods of moving an idea from the laboratory to market readiness and a more sophisticated pooling of re-sources. Thus, winning ideas and organizations prob-ably will be based on significant levels of cooperation both vertically (research, engineers, marketeers) as well as horizontally (between organizations nationally and internationally).

100,584

PB91-203182 Not available NTIS National Bureau of Standards, Gaithersburg, MD. Office of the Associate Director for Programs, Budget and Finance

Established Microwave Frequency Standards. Final rept.

H. Hellwig. 1989, 2p Pub. in Frequency Standards and Metrology, p44-45 1989.

Keywords: \*Frequency standards, Historical aspects, Atomic clocks, Ion storage, Microwaves, Rubidium, Cesium, Hydrogen, Masers, Reprints.

The paper is the introduction to a series of papers by other authors on 'established microwave frequency standards'. A historical background is given tracing the development of microwave frequency standards since the experiments by Stern-Gerlach in 1921. A brief summary of their salient technical features is given, followed by a discussion of performance and applications. Finally, the advent of a new contender, the mercury ion storage principle, is briefly described.

100,585

PB91-231605 PC A03/MF A01 National Inst. of Standards and Technology (NML), Boulder, CO. Time and Frequency Div.

NIST Time and Frequency Services. Special pub. (Final)

R. E. Beehler, and M. A. Lombardi. Jun 91, 32p NIST/SP-432

Also available from Supt. of Docs.

Keywords: \*Radio broadcasting, \*Frequency standards, \*Time signals, High frequency, Low frequency, Navigational aids, Computer networks, Voice communication, Air traffic control, GOES satellites, Calibratics U.S. MICH. tion, Uses, US NIST

NIST Time and Frequency Services (Special Publication 432 (Revised 1990)) is a revision of SP 432, last published in 1979. It describes services available, as of December 1990, from NIST radio stations WWV, WWVH, and WWVB; from GOES satellites; from Loran-C; by telephone (voice and modem); and from the NIST Frequency Measurement Service.

100,586

PB91-236950 Not available NTIS National Inst. of Standards and Technology (PL), Boulder, CO. Time and Frequency Div. Precise Ephemerides for GPS Time Transfer.

Final rept.

W. Lewandowski, and M. A. Weiss. 1988, 11p Pub. in Proceedings of Annual Precise Time and Time Interval (PTTI) Applications and Planning Meeting (21st), Redondo Beach, CA., November 28-30, 1990, p95-105 1988.

Keywords: \*Ephemeris time, Global positioning system, Precision, Comparison, Reprints, \*Broadcast ephemerides, \*Time transfer.

The present technology of atomic clocks motivates time transfer techniques with nanosecond accuracy. Global Positioning System (GPS), the most common means for international time comparisons could achieve such accuracy over short distances (up to 1000 km). Over intercontinental distances, the accuracy of the GPS time transfer ranges between 20 and 30 ns. Some of the principal error sources are the broadcast ephemerides, the broadcast ionospheric model, and the local antenna coordinates. The study investi-gates the quality of broadcast ephemerides by com-paring them with precise ephemerides and by using precise ephemerides for time transfer. Another aspect of the work is to suggest a strategy to overcome the planned degradation of GPS satellite messages via Selective Availability (SA).

100,587

PB92-123132 PC A03/MF A01 National Inst. of Standards and Technology, Boulder,

Time Domain Frequency Stability Calculated from the Frequency Domain Description: Use of the SIGINT Software Package to Calculate Time Domain Frequency Stability from the Frequency

F. L. Walls, J. Gary, A. O'Gallagher, R. Sweet, and L. Sweet, Sep 91, 39p NISTIR-89/3916-REV Supersedes PB90-257684.

Keywords: \*Frequency stability, Time domain, SIGINT computer code, Fortran 77 programming language, Frequency domain, Allan variance.

The authors describe the use of SIGINT, an interactive software package developed by the National Institute of Standards and Technology, which facilitates the cal-culation of time domain frequency stability from frequency domain data as a function of measuring time in terms of either the Allan variance (sigma squared(sub y))(tau); the modified Allan variance, mod(sigma squared(sub y))(tau); or (sigma squared(sub y))(tau) = (tau/(square root of 3))mod(sigma y)/(tau) = (tau) (square 100t of 100t sor. It also runs on many other systems; however, calls to an available graphics library will need to be substi-tuted for those that are included in this version. The program uses either a user defined function for the nput noise or default functions that describe the noise types commonly found in oscillators, amplifiers, frequency multipliers, frequency dividers, and general signal processing equipment including up to four coherent bright lines in the noise spectra. These default functions make it simple to analyze the time domain frequency stability as a function of measuring band-width using realistic first-, second-, or third-order lowpass filters or the simplified infinitely sharp cutoff parameter. The default functions are also set up to examine the effect of various servo parameters on the performance of a frequency source locked to a frequency reference.

### Radio & Television Equipment

100.588

PB91-134874 Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Time and Frequency Div.

Extending the Range and Accuracy of Phase Noise Measurements

Final rept.

F. L. Walls, A. J. D. Clements, C. M. Felton, M. A. Lombardi, and M. D. Vanek. 1988, 10p Pub. in Proceedings of Symposium on Frequency Con-trol (42nd), Baltimore, MD., June 1-3, 1988, p432-441.

Keywords: Electrical measurement, Quartz resonators, Frequency stability, Oscillators, Accuracy, Reprints, \*Phase noise, Calibration.

The paper describes recent progress in extending high accuracy measurements of phase noise in oscillatoors and other devices for carrier frequencies from the rf to the millimeter region and Fourier frequencies up to 10% of the carrier (or a maximum of about 1 GHz). A brief survey of traditional precision techniques for measuring phase noise is included as a basis for comparing their relative performance and limitations.

100.589

PB91-134882 Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Time and Frequency Div.

Accuracy Model for Phase Noise Measurements.

F. L. Walls, C. M. Felton, A. J. D. Clements, and T. D. Martin. 1989, 16p Pub. in Proceedings of Annual Precise Time and Time Interval (PTTI) Applications and Planning Meeting (21st), Redondo Beach, CA., November 28-30, 1989, 205 210 p295-310.

Keywords: Microwave amplifiers, Microwave oscillators, Frequency synthesizers, Spectrum analyzers, Frequency stability, Electrical measurement, Accuracy, Reprints, \*Phase noise, Time domain, Calibration.

The authors have recently completed a new modular system for accurate measurements of phase noise in oscillators, amplifiers, frequency synthesizers, and passive components. This new system is capable of measuring the phase noise at carrier frequencies from 5 MHz to 1.5 GHz, 1.5 to 26 GHz, and 33 to 50 GHz. Other frequency ranges can be measured using external mixers to convert the signals into one of the above frequency ranges. The analysis bandwidths vary from 0.1 Hz to 10% of the carrier frequency up to a maximum of about 1 GHz. Extensive internal calibration of the system is used to correct for all gain variations with

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### Radio & Television Equipment

analysis frequency including phase-locked-loop and cable-loss effects. Detailed descriptions of the new calibration procedures, including a sample table of uncertainties, are given. High accuracy determinations of phase noise can be used to compute accurate values of short-term, time-domain frequency stability.

PB91-162040 Not available NTIS National Inst. of Standards and Technology (NEL), Boulder, CO. Electromagnetic Fields Div. Evaluation of Dual-Port Circularly

Polarized Probes for Planar Near-Field Measurements.

M. H. Francis, and K. MacReynolds, 1990, 6p. Pub. in Proceedings of Annual Meeting and Symposium on Antenna Measurement Techniques Association (12th), Philadelphia, PA., October 7-16, 1990, p13-3-13-8.

Keywords: \*Probes(Electromagnetic), Extremely high frequency, Millimeter waves, Near field, Circular polarization, Cross polarization, Gain, Reprints, \*Antenna measurements.

Accurate near-field cross-polarization measurements on circularly polarized (CP) antennas at millimeter-wave frequencies require well-characterized probes with low axial ratios. The authors have recently ob-tained and calibrated dual-port CP horns for use as near-field probes at frequencies of 40-50 GHz. The authors present some gain, axial ratio, and pattern measurements for these probes and show that they give accurate cross-polarization measurements.

100.591

PB91-162156 Not available NTIS National Inst. of Standards and Technology (NEL), Boulder, CO. Electromagnetic Fields Div. Microstrip Patch Antenna as a Standard Transmit-

ting and Receiving Antenna.

Final rept. M. Kanda, 1989, 3p

See also PB90-206038.

Pub. in Proceedings of International Symposium on Electromagnetic Compatibility, Nagoya, Japan, September 8-10, 1989, p460-462.

Keywords: \*Microstrip antennas, Antenna radiation patterns, Electrical impedance, Standards, Reprints, Patch antennas.

The paper discusses the possibility of employing a microstrip patch antenna as a standard transmitting and receiving antenna. The intrinsic properties of the substrate used for the antenna are determined by careful impedance measurements. The experimental results indicate that the transmitting characteristics of a microstrip antenna can be theoretically determined from its geometry. The microstrip patch antenna discussed here is physically small (20 cm square for 450 MHz) and can be well matched to a power delivery system (SWR = 1.17).

### Verbal

100,592

PB91-189910 Not available NTIS National Inst. of Standards and Technology (NCSL), Gaithersburg, MD. Advanced Systems Div. Phone-Mediated Word Alignment for Speech Recognition Evaluation.

Final rept.

J. Picone, G. R. Doddington, and D. S. Pallett. 1990,

Pub. in IEEE (Institute of Electrical and Electronics Engineers) Transactions on Acoustics, Speech and Signal Processing 38, n3 p559-562 Mar 90.

Keywords: \*Speech recognition, \*Algorithms, Automation, Performance evaluation, Speech analysis, Re-

The paper presents an algorithm that produces a word-based alignment of two text strings by post-processing the output of a phone-based alignment procedure. The alignment is performed using an unconstrained endpoint dynamic optimization framework, and minimizes the readjustment of word boundaries as determined by the phone-level alignment.

100,593 PB91-195396 Not available NTIS National Bureau of Standards (ICST), Gaithersburg,

MD. Advanced Systems Div. Scoring Continuous Speech in the DARPA Speech

Recognition Program: Part 2. Final rept.

D. S. Pallett. 1988, 5p

Pub. in Proceedings of AVIOS '88 Voice I/O System Applications Conference, San Francisco, CA., October 4-6, 1988, p1-5.

Keywords: \*Speech recognition, \*Computer applications, \*Performance evaluation, Automation, Tests, Protocol, Computer software, Reprints.

The paper outlines considerations taken in developing and implementing Benchmark Test Procedures for evaluating the performance of large vocabulary continuous speech recognition systems using the DARPA Resource Management Speech Database. These tests were implemented in March and October 1987 and in June of 1988, with future tests planned using the same test protocol. The emphasis of the discussion in the paper is on scoring the results of the tests and includes a brief discussion of results obtained using scoring software.

100.594

PB91-505370 CD-ROM\$1200.00 National Inst. of Standards and Technology (CSL), Gaithersburg, MD. Automated Speech Recognition

DARPA Air Travel Information System (ATISO) Speaker-Dependent Training Data (on CD-ROM).

Data file.

Nov 90, CD-ROM NIST/DF/VD-91/003

Microsoft Extension version 2.1. User instructions on disc 'readme.doc'. See also PB91-505362, PB91-505364, PB90-501776, PB89-226666, PB90-500547, PB91-505065, PB91-506592, and PB90-500539. The datafile is on four, 4.72 inch discs.

Keywords: \*Data file, \*Speech recognition, Training, Air traffic, Information systems, Acoustics, Models, Microphones, CD-ROM.

The set of discs is the third release in a series of CD-ROMs containing recordings of speech in the DARPA Air Travel Information System (ATIS) domain. The set contains 'read' speech intended to permit acoustic modelling for 10 of the speakers of an earlier release (CD5-1.1) in the series, and can be used in training speaker-dependent speech recognition systems. Discs 5-3.1 and 5-4.1 contain speech data for the close-talking (Sennheiser) microphone, and 5-5.1 and 5-6.1 contain data for the desk-top (Crown PCC-160) microphone. The set of CD-ROMs augments material on two earlier releases, PB91-505354 and PB91-505362. The first release contains spontaneous utterances elicited in a 'Wizard-of-Oz' simulation of a spoken language system capable of providing air travel information derived from a simplified version of the Official Airline Guide, along with the relational data-base containing the travel information. The second re-lease contains 'read' versions of the spontaneous utterances for 20 of the speakers, along with 40 adaptation utterances for each of these speakers.

100.595

PB91-509802 CD-ROM\$500.00 National Inst. of Standards and Technology (CSL), Gaithersburg, MD. Automated Speech Recognition

Road Rally Conversational Speech Corpora (on CD-ROM).

Data file. Sep 91, CD-ROM NIST/DF/VD-91/015

System: Sun Microsystems 3/180; OS 4.1 operating system. Microsoft Extension Version 2.1. No color requirement or hard disk required. 'Readme.doc' on Disc. Software is written in 'C' Source Code. See also PB89-226666, PB90-501776, PB90-500539, PB91-505362, PB91-505354, PB90-500547, PB91-505065 and PB91-506592.

The datafile is on one, 4.72 inch disc. Data format: ISO

\*Speech Keywords: \*Data file, \*Speech recognition, Words(Language), Planning, CD-ROM, Conversation, Road rallys.

The 'Road Rally' corpora were designed for the development and testing of word-spotting systems and were collected in a conversational domain using a road rally planning task as the topic. The corpora actually consists of two sub-corpora, 'Stonehenge' and 'Waterloo'. The Stonehenge corpus contains road rally planning conversations as well as some read speech collected using high quality microphones and a telephone-simulating filter. The Waterloo corpus contains read speech in a road rally planning domain collected using actual telephone lines.

# COMPUTERS, CONTROL & INFORMATION THEORY

### **Computer Hardware**

100.596

N91-25793/1

(Order as N91-25755/0, PC A99/MF A04) National Inst. of Standards and Technology (NML), Boulder, CO. Time and Frequency Div. Synchronizing Computer Clocks Using a Local

Area Network. J. Levine. May 90, 9p

Pub. in Proceedings of Annual Precise Time and Time Interval (PTTI) Applications and Planning Meeting (22nd) p409-417 (See N91-25755 17-70).

Keywords: Calibrating, \*Clocks, \*Local area networks, \*Time measurement, Protocol (Computers), Telephones, \*Computer networks, \*Synchronism.

Researchers completed the first tests of a method to synchronize the clocks of networked computers to the National Institute of Standards and Technology (NIST) time scale. The method uses a server computer to dis seminate the time to other clients on the same local-area network. The server is synchronized to NIST using the ACTS protocol over a dial-up telephone line. The software in both the server and the parameters of this model are used to adjust the time of the local clock and the interval between calibration requests in a statistically optimum way. The algorithm maximizes the time between calibrations while at the same time keeping the time of the local clock correct within a specific tolerance. The method can be extended to synchronize computers linked over wide-area networks, and an experiment to test the performance of the algorithms over such networks is being planned.

100,597

Final rept.

PB91-147652 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Mathematical Analysis Div. Closure and Precision in Level-Index Arithmetic.

D. W. Lozier, and F. W. J. Olver. 1990, 10p Pub. in SIAM (Society for Industrial and Applied Mathematics) Jnl. of Numerical Analysis 27, n5 p1295-1304

Keywords: \*Arithmetic units, \*Computer systems hardware, Numerical precision, Error analysis, Computer calculations, Floating point arithmetic, Reprints.

First it is proved that two recently introduced systems of computer arithmetic, the level-index (li) and symmetric level-index (sli) systems are closed under the four basic arithmetic operations, provided that division by zero is excluded and the operations are executed in finite precision. In consequence, the li and sli systems are free from the defects of overflow and underflow. Second, measures of precision are discussed and compared. Third, the ranges and local precisions of numbers stored in the li and sli systems are compared with corresponding ranges and local precisions of numbers stored in the floating-point system.

100,598

Not available NTIS PB91-147660 National Inst. of Standards and Technology (ICST), Gaithersburg, MD. Advanced Systems Div.

### Computer Hardware

Workloads, Observables, Benchmarks and Instrumentation.

Final rept.

G. Lyon, and R. D. Snelick. 1990, 12p

See also PB90-207770. Pub. in Proceedings of Joint International Conference on Vector and Parallel Processing, Zurich, Switzerland, September 10-13, 1990, p86-97.

Keywords: \*Computer systems performance, \*Performance evaluation, Benchmarks, Comparison, Trees(Mathematics), Observation, Work measurement, Reprints, Workloads.

A compact user-level summary, a use-tree, explains system variabilities across benchmarks. The tree provides a clear, static declaration of the relationships among a limited number of major system resources that determine most performance variance. The new approach is especially effective with hardware instrumentation that decouples workload from observation (otherwise, a compact set of observables may be unavailable). A tree supports simple predictions and promotes more meaningful comparisons of workloads. Accounting for the sources of performance variation shown in the tree can inspire new methods of assess-ment; a 'time dilation' technique illustrates this for loosely-coupled systems with local clocks.

100,599 PB91-158766 Not available NTIS National Bureau of Standards (ICST), Gaithersburg, MD. Systems and Software Technology Div. 1987: The Year of the 386.

Final rept.

A. L. Hankinson. 1988, 2p Pub. in IEEE (Institute of Electrical and Electronics Engineers) Spectrum 25, n1 p32-33 Jan 88.

Keywords: \*Personal computers, \*Chips(Electronics), Workstations, Microcomputers, Computer software, Reprints, Intel 80386 computers.

Users of personal computers will likely remember 1987 as the year of the Intel 80386. This chip had a major influence on the three themes that characterized the significant PC related milestones during 1987. The first theme is the convergence of PC's and engineering workstations. The second theme is the blurring of the distinction between software for PC's minicomputers and mainframes. The final theme is the end of the era of the 'safe buy'. Each of these themes is presented in the context of the significant PC related milestones that occurred during 1987.

100,600

PB91-158899 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Factory Automation Systems Div. Choosing a Name for Your Computer.

Final rept. D. Libes. 1990, 8p

Pub. as Choosing a Name for Your Computer, p1-8 Aug 90.

Keywords: \*Computers, Guidelines, Reprints, \*Domain name system, Hostname, Computer name. Keywords:

In order to easily distinguish between multiple computers, the author's give them names. Experience has taught that it is as easy to choose bad names as it is to choose good ones. The essay presents guidelines for deciding what makes a name good or bad.

100,601 PB91-159319 Not available NTIS National Inst. of Standards and Technology (ICST), Gaithersburg, MD. Advanced Systems Div. Hardware Instrumentation Approach for Performance Measurement of a Shared-Memory Multi-

processor. Final rept.

G. Nacht, and A. Mink. 1989, 16p See also PB89-186852. Sponsored by Defense Advanced Research Projects Agency, Arlington, VA.
Pub. in Proceedings of International Conference on
Modeling Techniques and Tools for Computer Performance Evaluation (4th), Palma, Spain, September
14-16, 1988, p249-264

Keywords: \*Multiprocessors, \*Computer performance evaluation, Parallel processors, Measuring instruments, Computer systems hardware, Reprints

Two approaches for the design of performance measurement instrumentation for a shared memory, tightly

coupled, MIMD multiprocessor are presented. The TRAce Measurement System (TRAMS) is a hybrid measurement tool used to obtain trace measurement information. The Resource Measurement System (REMS) is a non-intrusive hardware measurement tool used to obtain both trace measurement and resource utilization information. The TRAMS approach provides a hardware assist to the more traditional software approach of obtaining timestamps from the operating system at each event to be measured. The hardware assist reduces the artifact that is introduced in a test program and is a feasible and economical approach to providing measurement capabilities to a wide range of multiprocessors. Manufacturers could offer this type of measurement tool as a plug-in option. The REMS approach provides more detailed and extensive measurement information than does the TRAMS approach and introduces no artifact to the test program, but it does this at a significantly higher cost. When access to pertinent signals is restricted the applicability of such a hardware tool is limited.

100,602 PB91-189894 Not available NTIS Mational Inst. of Standards and Technology (NCSL), Gaithersburg, MD. Advanced Systems Div. Conformance Tester for X.25 DTE Implementa-

Final rept.
H. Peng, D. H. Su, and S. A. Wakid. 1989, 4p
Pub. in IEEE (Institute of Electrical and Electronics Engineers) Network Magazine 3, n4 p27-30, 39, Jul 89.

Keywords: Standards, Tests, Reprints, \*Data terminal equipment, Defense Data Network, C programming language, Protocols.

A validation suite is presented to test the conformance of Data Terminal Equipment (DTE) to the ISO International Standard of the 1984 X.25 protocol (ISO 7776 and 8208) as well as to the CCITT recommendations of the 1980 version of the protocol. The test cases are based on ISO 8882 and the testing methodology itself complies with ISO 9646. The paper describes the design, instrumentation, and execution of this tester which is written in 'C' and available in the public domain.

PB91-201822 PC A05/MF A01 National Inst. of Standards and Technology (NCSL), Gaithersburg, MD. National Computer Systems Laboratory Annual

E. Lennon, S. Radack, and R. Roach. Dec 90, 76p NISTIR-4492

Also available from Supt. of Docs.

Keywords: \*Computers, \*Computer software, Information systems, Systems engineering, Computer security, Computer networks, Computer architecture, Telecommunication, Technology transfer, Federal informa-tion processing standards, \*National Computer Sys-tems Laboratory.

The report describes the annual computer and related telecommunications activities and accomplishments of the National Computer Systems Laboratory (NCSL). Following the Director's Foreword, an overview of the Laboratory is presented, including a current NCSL Organization Chart and selected staff accomplishments. Overviews of NCSL's five technical divisions are featured, followed by a section on Technology Transfer which details the vehicles NCSL uses to disseminate research and information to the public and technical communities. A list of Federal Information Processing Standards (FIPS) and FIPS order information conclude the annual report.

100,604 PB92-108950 PC A04/MF A01 National Inst. of Standards and Technology (EEEL), Gaithersburg, MD. Electricity Div. Video Processing with the Princeton Engine at NIST.

Technical note (Final). B. F. Field, and C. Fenimore. Aug 91, 54p NIST/TN-1288

Also available from Supt. of Docs. as SN003-003-03091-1.

Keywords: \*Image processing, \*Supercomputers Computer aided design, Computer architecture, Paral-\*Supercomputers. lel computers, Real time operations, Data compression, Modules, Fortran, \*Princeton Engine, Video processing, SIMD(Computers). The document describes the NIST program in digital processing, including a newly created Image Processing Laboratory at NIST that is available to governmental, industrial, and academic researchers working on digital image processing. The centerpiece of the laboratory is a video supercomputer, the Princeton Engine, designed and constructed by the David Sarnoff Research Center. The engine provides real-time video and image-processing capability, accepting a variety of video formats over multiple wideband input channels and outputting real-time video for immediate viewing. Because the Engine is programmable, it is possible to use it to evaluate prototypes of image processing com-ponents rapidly and efficiently. The hardware capabili-ties of the Princeton Engine are described as well as the available supporting video equipment in the Laboratory. Two programming examples are included to demonstrate the unusual programming environment and 'language' used to program the Engine. Appendices list the available predefined library modules, and the processor assembly language instructions.

100,605 PB92-116409 PC A05/MF A01 National Inst. of Standards and Technology (NCSL), Gaithersburg, MD. Advanced Systems Div

Test Methods for Optical Disk Media Characteristics (for 356 mm Ruggedized Magneto-optic Media).

Special pub.

Special pub.
F. L. Podio. Sep 91, 79p NIST/SP-500/191
Also available from Supt. of Docs. as SN003-003-03103-8. Sponsored by National Aeronautics and Space Administration, Hampton, VA. Langley Research Center.

Keywords: \*Tests, \*Computer storage devices, \*Optical disks, Optical data storage materials, Environmental tests, Radiation tests, Substrates, Standards, Magneto-optic media.

Standard test methods for computer storage media characteristics are essential and allow for conformance verification to media interchange standards. Tests methods are also needed to develop procedures which would allow for repeatability of results among different industry and U.S. Government sites. The test procedures documented in the publication reflect the work done by the NIST/NASA Working Group for the Development of Test Methods and Specifications for 356 mm Ruggedized Rewritable Media. The test methods were developed for 356 mm two-sided laminated glass substrate with a magneto-optic active layer media technology. These test methods may be used for testing other media types, but in each case their applicability must be evaluated. Test methods are included for a series of different media characteristics including: operational, non-operational, and storage environments, mechanical and physical characteristics, and substrate, recording layer, and preformat characteristics. Tests for environmental qualification and media lifetimes are also included. The test methods include testing conditions, testing procedures, a description of the testing setup, and the required calibration procedures.

100.606 PB92-123124 PC A05/MF A01 National Inst. of Standards and Technology (CSL), Gaithersburg, MD. Advanced Systems Div.
Monitoring and Reporting Techniques for Error
Rate and Error Distribution in Optical Disk Sys-

Final rept

F. L. Podio. Oct 91, 92p NIST/SP-500/198 Also available from Supt. of Docs. as SN003-003-03125-9. Proceedings of a workshop held in Colorado Springs, Colorado on August 5, 1991.

Keywords: \*Optical disks, \*Meetings, State of the art, Mechanical drives, Error analysis, Recommendations, Error detection, Error correction.

The report constitutes the proceedings of the workshop on Monitoring and Reporting Techniques for Error Rate and Error Distribution in Optical Disk Systems held on August 5, 1991, in Colorado Springs, Colorado. The objectives of the workshop were to identify the state of the art on error rate monitoring and reporting techniques in optical disk systems and to promote discussions on possible future implementations. The workshop presentations included the description of a Computer Systems Laboratory of the National Institute of Standards and Technology (CSL/NIST) program for investigating error reporting capabilities of optical disk

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drives, Federal Government needs on error detection, correction and reporting, and the state of the art on error reporting capabilities in current generation drives. Presentations also included the description of the capabilities of error correction and detection current chips and discussions on error management stratechips and discussions on error management strategies. During a discussion panel, the participants identified a preliminary set of user requirements and it was suggested that a Government/industry working group be organized in order to document a consensus positional production. tion between the Federal Government and industry in error reporting capabilities for future generation drives.

### Computer Software

100,607 AD-A233 961/2 PC A04/MF A01 National Inst. of Standards and Technology, Gaithers-

Ada Compiler Validation Summary Report. Certificate Number: 901109S1.11053, Digital Equipment Corporation VAX Ada, Version 2.2 VAX 8800 = > VAX 8800. Final rept.

12 Dec 90, 59p Rept no. AVF-NIST90DEC505-1-1.11

Keywords: \*Ada programming language, \*Compilers, \*Validation summary reports, Standards, Tests.

The Ada implementation described above was tested according to the Ada Validation Procedure (Pro90) against the Ada Standard (Ada83) using the current Ada Compiler Validation Capability (ACVC). This Validation Summary Report (VSR) give an account of the testing of this Ada implementation.

100,608 AD-A234 083/4 PC A05/MF A01 National Inst. of Standards and Technology, Gaithers-

burg, MD.
Ada Compiler Validation Summary Report: DDC International A/S, DACS VAX/VMS to 80186 Bare Ada Cross Compiler System, Version 4.6, VAX 8530 (Host) to Bare Board iSBC 186/93A (Host), 901129\$1.11079. Final rept.

30 Nov 90, 98p Rept no. NIST-90DDC500-8-1.11

Keywords: \*Ada programming language, \*Compilers, \*Validation summary reports, Standards, Tests.

The Ada implementation described above was tested according to the Ada Validation Procedures Pro90 against the Ada Standard Ada83 using the current Ada Compiler Validation Capability (ACVC). This Validation Summary Report (VSR) gives an account of the testing of this Ada implementation.

100,609 AD-A234 118/8 PC A06/MF A01 National Inst. of Standards and Technology, Gaithers-

Ada Compiler Validation Summary Report: Certificate Number: 901129S1.11112 DDC International A/S DACS 80386 DMS/OS Ada Compiler System, Version 4.6 IBM PS/2 Model 80-311 = > IBM PS/2 Model 80-311. Final rept.

30 Nov 90, 117p Rept no. NIST90DDC500-9-1.11

Keywords: \*Ada programming language, \*Compilers, \*Validation summary reports, Standards, Tests.

The Ada implementation described above was tested according to the Ada Validation Procedures (Pro90) against the Ada Standard (Ada83) using the current Ada Compiler Validation Capability (ACVC). This Validation Summary Report (VSR) gives an account of the testing of this Ada implementation.

100,610 AD-A234 323/4 PC A04/MF A01 National Inst. of Standards and Technology, Gaithers-

Ada Compiler Validation Summary Report: Certificate Number: 901129S1.11050 DDC International A/S DACS VAX/VMS Native Ada Compiler System, Version 4.6 VAX 8530 = > VAX 8530. 30 Nov 90, 53p

Keywords: \*Ada programming language, \*Compilers, \*Validation summary reports, Standards, Tests.

The Ada implementation described above was tested according to the Ada Validation Procedures Pro90 against the Ada Standard Ada83 using the current Ada Compiler Validation Capability (ACVC). This Validation Summary Report (VSR) gives an account of the testing of this Ada implementation.

100 61: AD-A234 350/7 PC A04/MF A01 National Inst. of Standards and Technology, Gaithers-

burg, MD.
Ada Compiler Validation Summary Report: Digital Equipment Corporation, VAX Ada, Version 2.2, BAX 8800 (Host) t VAX MicroVAX II Running VAXELN Version 4.1 (Target), 901109S1.11054. Final rept.

12 Dec 90, 59p Rept no. NIST-90DEC505-2-1.11

Keywords: \*Ada programming language, \*Compilers, \*Validation summary reports, Standards, Tests.

The Ada implementation described above was tested according to the Ada Validation Procedures Pro90 against the Ada Standard Ada83 using the current Ada Compiler Validation Capability (ACVC). This Validation Summary Report (VSR) gives an account of the testing of this Ada implementation.

AD-A234 380/4 PC A03/MF A01 National Inst. of Standards and Technology, Gaithersburg, MD.

Ada Compiler Validation Summary Report: Certificate Number: 901129S1.11051, DDC International A/S, DACS VAX/VMS to 68020 Bare Cross Compiler System, Version 4.6 MicroVAX 3100 Greater Than or Equal to Motorola MVME133. Final rept. 17 Dec 90-1 Mar 91.

1 Mar 91, 45p

Keywords: \*Ada programming language, \*Compilers, \*Validation summary reports, Standards, Tests.

The Ada implementation described above was tested according to the Ada Validation Procedures Pro 90 against the Ada Standard Ada 83 using the current Ada Compiler Validation Capability (ACVC). This Validation Capability (ACVC). dation Summary Reports (VCR) gives an account of the testing of this data implementation.

100,613 AD-A234 438/0 PC A06/MF A01 National Inst. of Standards and Technology, Gaithers-

Durg, MD.
Ada Compiler Validation Summary Report: Certificate Number: 901129S1.11077 DDC International A/S DACS VAX/VMS to 80186 Bare Ada Cross Compiler System with Rate Monotonic Scheduling, Version 4.6 VAX 8530 => Bare Board iSBC/03A. Final rept. 30 Nov 90, 101p

Keywords: \*Ada programming language, \*Compilers, \*Validation summary reports, Standards, Tests.

The Ada implementation described above was tested according to the Ada Validation Procedures (Pro 90) against the Ada Standard (Ada 83) using the current Ada Compiler Validation Capability (ACVC). This Validation Summary Report (VSR) gives an account of the testing of this Ada implementation.

100.614 AD-A234 439/8 PC A04/MF A01 National Inst. of Standards and Technology, Gaithers-

burg, MD.

Ada Compiler Validation Summary Report: Certificate Number: 901129S1.11075 DDC International A/S DACS 80386 UNIX V Ada Compiler System, Version 4.6 ICL DRS300 => ICL DRS300. Final rept.

30 Nov 90, 72p

Keywords: \*Ada programming language, \*Compilers, \*Validation summary reports, Standards, Tests.

The Ada implementation described above was tested according to the Ada Validation Procedures Pro90 against the Ada Standard Ada83 using the current Ada Compiler Validation Capability (ACVC). This Validation Summary Report (VSR) gives account of the testing of this Ada implementation.

100,615 AD-A234 529/6

PC A06/MF A01

National Inst. of Standards and Technology, Gaithersburg, MD.

bold, Mo.
Ada Compiler Validation Summary Report: Certificate Number: 901129S1.11074 DDC International A/S DACS VAX/VMS 60 80386 PM Bare Ada Cross Compiler System, Version 4.6 VAX 8530 => Bare Board iSBC 386/21.

Final rept. 30 Nov 90, 101p

Keywords: \*Ada programming language, \*Compilers, \*Validation summary reports, Standards, Tests.

The Ada implementation described above was tested according to the Ada Validation Procedures Pro90 against the Ada Standard Ada83 using the current Ada Compiler Validation Capability (ACVC). This Validation Summary Report (VSR) gives an account of the testing of this Ada implementation.

100,616 AD-A239 715/6 PC A06/MF A02 National Inst. of Standards and Technology (NCSL), Gaithersburg, MD. Software Standards Validation

Ada Compiler Validation Summary Report. Certifi-cate Number: 910510S1.11161 UNISYS Corpora-tion, UCS Ada, Version 1R1, 2200/600 (Host and Target). Revision.

Final rept. 24 Jul 91, 123p Revision of report dated 9 Apr-10 May 91.

Keywords: \*Ada programming language, \*Compilers, Standardization, Test and evaluation, Computers, Computer program verification, \*Validation summary

This Validation Summary Report describes the extent to which a specific Ada compiler conforms to the Ada Standard, ANSI/MIL-STD-1815A. This report explains all technical terms used within it and thoroughly reports the results of testing this compiler using the Ada Compiler Validation Capability. An Ada compiler must be implemented according to the Ada Standard, and any implementation-dependent features must conform to the requirements of the Ada Standard. The Ada Standard must be implemented in its entirety, and nothing can be implemented that is not in the Standard must be implemented that it is not in the Standard must be implem ard. Even though all validated Ada compilers conform to the Ada Standard, it must be understood that some differences do exist between implementations. The Ada Standard permits some implementation dependencies--for example, the maximum length of identifiers or the maximum values of integer types. Other differences between compilers result from the characteristical tics of particular operating systems, hardware, or implementation strategies. All the dependencies observed during the process of testing this compiler are given in this report. The information in this report is derived from the test results produced during validation testing. The validation process includes submitting a suite of standardized tests, the ACVC, as inputs to an Ada compiler and evaluating the results.

100,617 AD-A240 511/6 PC A05/MF A01 National Inst. of Standards and Technology, Gaithersburg, MD.

Ada Compiler Validation Summary Report: Certificate Number: 910626S1.11179 U.S. Navy Ada/M, Version 4.0 (OPTIMIZE) VAX 11/785 => AN/AYK-14 (Bare Board).

Finàl rept. 30 Jul 91, 89p

Keywords: \*Ada programming language, \*Compilers, Standardization, Test and evaluation, \*Validation summary reports.

This Validation Summary Report describes the extent to which a specific Ada compiler conforms to the Ada Standard, ANSI/MIL-STD-1815A. This report explains all technical terms used within it and thoroughly reports the results of testing this compiler using the Ada Compiler Validation Capability. An Ada compiler must be implemented according to the Ada Standard, and any implementation-dependent features must conform to the requirements of the Ada Standard. The Ada Standard must be implemented in its entirety, and nothing can be implemented that is not in the Standard. Even though all validated Ada compilers conform to the Ada Standard, it must be understood that some differences do exist between implementations. The Ada Standard permits some implementation depend-

### **Computer Software**

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100,618
AD-A240 512/4
PC A04/MF A01
National Inst. of Standards and Technology, Gaithersburg, MD.
Ada Compiler Validation Summary Report: Certifi-

Ada Compiler Validation Summary Report: Certificate Number 910705S1.11192 InterAct Corporation InterAct Ada Mips Cross-Compiler System, Release 2.0 MicroVAX 3100 Cluster = > Lockheed Sanders STAR MVP R3000/R3010 board (Bare Machine).

Final rept. 31 Jul 91, 63p

Keywords: \*Ada programming language, \*Compilers, Standardization, Test and evaluation, \*Validation summary reports.

This Validation Summary Report describes the extent to which a specific Ada compiler conforms to the Ada Standard, ANSI/MIL-STD-1815A. This report explains all technical terms used within it and thoroughly reports the results of testing this compiler using the Ada Compiler Validation Capability. An Ada compiler must be implemented according to the Ada Standard, and any implementation-dependent features must conform to the requirements of the Ada Standard. The Ada Standard must be implemented in its entirety, and nothing can be implemented that is not in the Standard. Even though all validated Ada compilers conform to the Ada Standard, it must be understood that some differences do exist between implementations. The Ada Standard permits some implementation dependencies—for example, the maximum length of identifiers or the maximum values of integer types. Other differences between compilers result from the characteristics of particular operating systems, hardware, or implementation strategies. All the dependencies observed during the process of testing this compiler are given in this report. The information in this report is derived from the test results produced during validation testing. The validation process includes submitting a suite of standardized tests, the ACVC, as inputs to an Ada compiler and evaluating the results.

100,619
AD-A240 610/6
PC A03/MF A01
National Inst. of Standards and Technology, Gaithers-

Ada Compiler Validation Summary Report: Certificate Number: 910502S1.11158 DDC International A/S, DACS VAX/VMS to 80860 Bare Ada Cross Compiler System, Version 4.6.1, VAX 8530 (Host) to Tadpole Technology PLC TP860M (Bare Board)

Final rept. 24 Jul 91, 36p

Keywords: \*Ada programming language, \*Compilers, Standardization, Test and evaluation, \*Validation summary reports.

This Validation Summary Report describes the extent to which a specific Ada compiler conforms to the Ada Standard, ANSI/MIL-STD-1815A. This report explains all technical terms used within it and thoroughly reports the results of testing this compiler using the Ada Compiler Validation Capability. An Ada compiler must be implemented according to the Ada Standard, and any implementation-dependent features must conform to the requirements of the Ada Standard. The Ada Standard must be implemented in its entirety, and nothing can be implemented that is not in the Standard. Even though all validated Ada compilers conform to the Ada Standard, it must be understood that some differences do exist between implementations. The Ada Standard permits some implementation dependencies—for example, the maximum length of identifiers or the maximum values of integer types. Other differences between compilers result from the characteristics of particular operating systems, hardware, or implementation strategies. All the dependencies observed during the process of testing this compiler are given in this report. The information in this report is derived from the ets results produced during valida-

tion testing. The validation process includes submitting a suite of standardized tests, the ACVC, as inputs to an Ada compiler and evaluating the results.

100.620

AD-A240 611/4 PC A05/MF A01 National Inst. of Standards and Technology, Gaithersburg, MD.

Durg, MD.
Ada Compiler Validation Summary Report: Certificate Number: 910626S1.11176 U.S. Navy, Ada/L, Version 4.0 (/Optimize), VAX 11/785 (Host) to AN/UYJ-43 (Single CPU) (Bare Board) (Target). Final rept.

30 Jul 91, 79p

Keywords: \*Ada programming language, \*Compilers, Standardization, Test and evaluation, \*Validation summary reports.

This Validation Summary Report describes the extent to which a specific Ada compiler conforms to the Ada Standard, ANSI/MIL-STD-1815A. This report explains all technical terms used within it and thoroughly reports the results of testing this compiler using the Ada Compiler Validation Capability. An Ada compiler must be implemented according to the Ada Standard, and any implementation-dependent features must conform to the requirements of the Ada Standard. The Ada Standard must be implemented in its entirety, and nothing can be implemented that is not in the Standard. Even though all validated Ada compilers conform to the Ada Standard, it must be understood that some differences do exist between implementations. The Ada Standard permits some implementation dependencies-for example, the maximum length of identifiers or the maximum values of integer types. Other differences between compilers result from the characteristics of particular operating systems, hardware, or implementation strategies. All the dependencies observed during the process of testing this compiler are given in this report. The information in this report is derived from the test results produced during validation testing. The validation process includes submitting a suite of standardized tests, the ACVC, as inputs to an Ada compiler and evaluating the results.

100,621

AD-A240 612/2 PC A05/MF A01 National Inst. of Standards and Technology, Gaithersburg, MD.

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Final rept. 30 Jul 91, 89p

Keywords: \*Ada programming language, \*Compilers, Standardization, Test and evaluation, \*Validation summary reports.

This Validation Summary Report describes the extent to which a specific Ada compiler conforms to the Ada Standard, ANSI/MIL-STD-1815A. This report explains all technical terms used within it and thoroughly reports the results of testing this compiler using the Ada Compiler Validation Capability. An Ada compiler must be implemented according to the Ada Standard, and any implementation-dependent features must conform to the requirements of the Ada Standard. The Ada Standard must be implemented in its entirety, and nothing can be implemented that is not in the Standard. Even though all validated Ada compilers conform to the Ada Standard, it must be understood that some differences do exist between implementations. The Ada Standard permits some implementation dependencies-for example, the maximum length of identifiers or the maximum values of integer types. Other differences between compilers result from the characteristics of particular operating systems, hardware, or implementation strategies. All the dependencies observed during the process of testing this compiler are given in this report. The information in this report is derived from the test results produced during validation testing. The validation process includes submitting a suite of standardized tests, the ACVC, as inputs to an Ada compiler and evaluating the results.

100,622

AD-A240 613/0 PC A05/MF A01 National Inst. of Standards and Technology, Gaithersburg, MD. Ada Compiler Validation Summary Report: Certificate Number: 910626S1.11175 U.S. Navy Ada/M, Version 4.0 (/Optimize), VAX 8550 (Host) to AN/AYK-14 (Bare Board) (Target). Final rept.

30 Jul 91, 87p

Keywords: \*Ada programming language, \*Compilers, Standardization, Test and evaluation, \*Validation summary reports.

This Validation Summary Report describes the extent to which a specific Ada compiler conforms to the Ada Standard, ANSI/MIL-STD-1815A. This report explains all technical terms used within it and thoroughly reports the results of testing this compiler using the Ada Compiler Validation Capability. An Ada compiler must be implemented according to the Ada Standard, and any implementation-dependent features must conform to the requirements of the Ada Standard. The Ada Standard must be implemented in its entirety, and nothing can be implemented that is not in the Standard. Even though all validated Ada compilers conform to the Ada Standard, it must be understood that some differences do exist between implementations. The Ada Standard permits some implementation dependencies-for example, the maximum length of identifiers or the maximum values of integer types. Other differences between compilers result from the characteristics of particular operating systems, hardware, or implementation strategies. All the dependencies observed during the process of testing this compiler are given in this report. The information in this report is derived from the test results produced during validation testing. The validation process includes submitting a suite of standardized tests, the ACVC, as inputs to an Ada compiler and evaluating the results.

100.623

AD-A240 762/5 PC A04/MF A01 National Inst. of Standards and Technology, Gaithersburg, MD.

Ada Compiler Validation Summary Report. Certificate Number: 910705S1.11191, InterACT Corporation InterACT Ada 1750A Compiler System, Release 3.5, MicroVAX 3100 Cluster => InterACT MIL-STD-1750A Instruction Set Architecture Simulator, Release 2.3 (Bare Machine).

Final rept. 31 Jul 91, 75p

Keywords: \*Ada programming language, \*Compilers, Computer program verification, \*Validation summary reports, Standardization, Test and evaluation.

The Ada implementation described above was tested according to the Ada Validation Procedures (Pro90) against the Ada Standard (Ada83) using the current Ada Compiler Validation Capability (ACVC). This Validation Summary Report (VSR) gives an account of the testing of this Ada implementation. For any technical terms used in this report, the reader is referred to Pro90. A detailed description of the ACVC may be found in the current ACVC User's Guide (UG89).

100,624

AD-A240 763/3 PC A05/MF A01 National Inst. of Standards and Technology, Gaithersburg, MD.

Ada Compiler Validation Summary Report. Certificate Number: 91062681.11178, U.S. Navy Ada/M, Version 4.0 (/OPTIMIZE) VAX 11/785 => AN/UYK-44 (EMR) (Bare Board).

Final rept. 30 Jul 91, 89p

Keywords: \*Ada programming language, \*Compilers, Computer program verification, \*Validation summary reports, Standardization, Test and evaluation.

The Ada implementation described above was tested according to the Ada Validation Procedures (Pro90) against the Ada Standard (Ada83) using the current Ada Compiler Validation Capability (ACVC). This Validation Summary Report (VSR) gives an account of the testing of this Ada implementation. For any technical terms used in this report, the reader is referred to Pro90. A detailed description of the ACVC may be found in the current ACVC User's Guide (UG89).

100,625

AD-A240 783/1 PC A05/MF A01 National Inst. of Standards and Technology, Gaithersburg, MD.

### Computer Software

Ada Compiler Validation Summary Report: Certificate Number 910626S1.11173 U.S. Navy Ada/L, Version 4.0 (/Optimize) VAX 855 = AN/UYK-43 (EMR) (Bare Board).

30 Jul 91, 80p

Keywords: \*Ada programming language, \*Compilers, Computer program verification, \*Validation summary reports, Standardization, Test and evaluation

The Ada implementation described above was tested according to the Ada Validation Procedures (Pro90) against the Ada Standard (Ada83) using the current Ada Compiler Validation Capability (ACVC). This Validation Summary Report (VSR) gives an account of the testing of this Ada implementation. For any technical terms used in this report, the reader is referred to Pro90. A detailed description of the ACVC may be found in the current ACVC User's Guide (UG89).

100,626 AD-A240 784/9 PC A05/MF A01 National Inst. of Standards and Technology, Gaithersburg, MD.

Ada Compiler Validation Summary Report: Certificate Number Number 910626S1.11172 U.S. Navy Ada/L, Version 4.0 (/Optimize) VAX 8550 = AN/ UYK-43 (Single CPU) (Bare Board).

Final rept. 30 Jul 91, 80p

Keywords: \*Ada programming language, \*Compilers, Computer program verification, \*Validation summary reports, Standardization, Test and evaluation.

The Ada implementation described above was tested according to the Ada Validation Procedures (Pro90) against the Ada Standard (Ada83) using the current Ada Compiler Validation Capability (ACVC). This Validation Summary Report (VSR) gives an account of the testing of this Ada implementation. For any technical terms used in this report, the reader is referred to Pro90. A detailed description of the ACVC may be found in the current ACVC User's Guide (UG89).

100.627 AD-A240 785/6 PC A03/MF A01 National Inst. of Standards and Technology, Gaithers-

burg, MD.
Ada Compiler Validation Summary Report: Certificate Number: 910502S1.11159 DDC International A/S DACS Sun-3/SunOS to 68030 Bare Ada Cross Compiler System, Version 4.6.4, MRI IEEE 695 (BASIC-MODE) Sun-3/50 = Motorola MVME143 Board (68030/68882).

Final rept. 24 Jul 91, 50p

Keywords: \*Ada programming language, \*Compilers, Computer program verification, \*Validation summary reports, Standardization, Test and evaluation.

The Ada implementation described above was tested according to the Ada Validation Procedures (Pro90) against the Ada Standard (Ada83) using the current Ada Compiler Validation Capability (ACVC). This Validation Summary Report (VSR) gives an account of the testing of this Ada implementation. For any technical terms used in this report the reader is referred to terms used in this report, the reader is referred to Pro90. A detailed description of the ACVC may be found in the current ACVC User's Guide (UG89).

AD-A240 849/0 PC A03/MF A01 National Inst. of Standards and Technology, Gaithers-

Ada Compiler Validation Summary Report. Certificate Number: 910502S1.11160 DDC International A/S DACS Sun-3/SunOS to 68030 Bare Ada Cross Compiler System, Version 4.6.4, MRI IEEE 695 (SECURE MODE) Sun-3/50 => Motorola MVME143 Board (68030/68882). Final rept.

24 Jul 91, 50p

Keywords: \*Ada programming language, \*Compilers, Security, Standardization, Test and evaluation, \*Validation summary reports, Computer program verifica-

This Validation Summary Report describes the extent to which a specific Ada compiler conforms to the Ada Standard, ANSI/MIL-STD-1815A. This report explains all technical terms used within it and thoroughly reports the results of testing this compiler using the Ada Compiler Validation Capability. An Ada compiler must be implemented according to the Ada Standard, and any implementation-dependent features must conform to the requirements of the Ada Standard. The Ada Standard must be implemented in its entirety, and nothing can be implemented that is not in the Standard. Even though all validated Ada compilers conform to the Ada Standard, it must be understood that some differences do exist between implementations. The Ada Standard permits some implementation dependencies--for example, the maximum length of identifiers or the maximum values of integer types. Other differences between compilers result from the characteristics of particular operating systems, hardware, or implementation strategies. All the dependencies observed during the process of testing this compiler are given in this report. The information in this report is derived from the test results produced during valida-tion testing. The validation process includes submitting a suite of standardized tests, the ACVC, as inputs to an Ada compiler and evaluating the results

100,629 AD-A240 850/8 PC A05/MF A01 National Inst. of Standards and Technology, Gaithersburg, MD.

Ada Compller Validation Summary Report. Certificate Number: 910626S1.11177 U.S. NAVY Ada/L, Version 4.0 (/OPTIMIZE) VAX 11/785 => AN/ UYK-43 (EMR) (Bare Board).

Final rept. 26 Jun 91, 80p

Keywords: \*Ada programming language, \*Compilers, Test and evaluation, \*Validation summary reports, Computer program verification, Standards.

This Validation Summary Report describes the extent to which a specific Ada compiler conforms to the Ada Standard, ANSI/MIL-STD-1815A. This report explains all technical terms used within it and thoroughly re ports the results of testing this compiler using the Ada Compiler Validation Capability. An Ada compiler must be implemented according to the Ada Standard, and any implementation-dependent features must conform to the requirements of the Ada Standard. The Ada Standard must be implemented in its entirety, and nothing can be implemented that is not in the Standard. Even though all validated Ada compilers conform to the Ada Standard, it must be understood that some differences do exist between implementations. The Ada Standard permits some implementation dependencies--for example, the maximum length of identifiers or the maximum values of integer types. Other differences between compilers result from the characteristics of particular operating systems, hardware, or implementation strategies. All the dependencies observed during the process of testing this compiler are given in this report. The information in this report is derived from the test results produced during validation testing. The validation process includes submitting a suite of standardized tests, the ACVC, as inputs to an Ada compiler and evaluating the results.

100,630 AD-A242 268/1 PC A08/MF A02 National Inst. of Standards and Technology, Gaithersburg, MD.

Ada Compller Validation Summary Report: Certificate Number: 910517S1.11163 U.S. Navy, AdaVAX, Version 5.0, (/NO OPTIMIZE) VAX 8350 (Host and Target). Final rept

17 May 91, 175p

No software available for distribution.

Keywords: \*Ada programming language, \*Compilers, Standardization, Test and evaluation, \*Validation summary reports, Computer program verification.

This Validation Summary Report describes the extent to which a specific Ada compiler conforms to the Ada Standard, ANSI/MIL-STD-1815A. This report explains all technical terms used within it and thoroughly reports the results of testing this compiler using the Ada Compiler Validation Capability. An Ada compiler must be implemented according to the Ada Standard, and any implementation-dependent features must conform to the requirements of the Ada Standard. The Ada to the requirements of the Ada Standard. The Ada Standard must be implemented in its entirety, and nothing can be implemented that is not in the Standard. Even though all validated Ada compilers conform to the Ada Standard, it must be understood that some differences do exist between implementations. The Ada Standard permits some implementation dependencies--for example, the maximum length of identifiers

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100,631 AD-A242 269/9 PC A05/MF A01 National Inst. of Standards and Technology, Gaithers-

burg, MD.
Ada Compiler Validation Summary Report: Certificate Number: 91051751.11162 U.S. Navy, AdaVAX, Version 5.0, (/OPTIMIZE) VAX 8600 (Host and Final rept.

17 May 91, 76p No software available for distribution.

Keywords: \*Ada programming language, \*Compilers, Standardization, Test and evaluation, \*Validation summary reports, Computer program verification.

This Validation Summary Report describes the extent to which a specific Ada compiler conforms to the Ada Standard, ANSI/MIL-STD-1815A. This reports the results of testing this compiler using the ADa Compiler Validation Capability. An Ada compiler must be implemented according to the Ada standard, and any implementation-dependent features must conform to the re-quirements of the Ada standard, the Ada Standard must be implemented in its entirety, and nothing can be implemented that is not in the standard. Even though all validated Ada compilers conform to the Ada Standard, it must be understood that some differences do exist between implementations. The Ada Standard oo exist between implementations. The Ada Standard permits some implementation dependencies—for example, the maximum length of identifiers or the maximum values of integer types. Other differences between compilers result from the characteristics of particular operating systems, hardward, or implementation strategies. All the dependencies observed during the process of testing this compiler are given in this report. The information in this report is derived from the test results produced during validation testing. The the test results produced during validation testing. The validation process includes submitting a suite of stand-ardized tests, the ACVC, as inputs to an Ada compiler and evaluating the results.

AD-A242 270/7 PC A04/MF A01 National Inst. of Standards and Technology, Gaithersburg, MD.

Ada Compiler Validation Summary Report: Certificate Number: 910517S1.11165 U.S. Navy, AdaVAX, Version 5.0 (/NO-OPTIMIZE), VAX 11/785 (Host and Target).

Final rept. 17 May 91, 72p No software available for distribution.

Keywords: \*Ada programming language, \*Compilers, Standardization, Test and evaluation, \*Validation summary reports, Computer program verification.

This Validation Summary Report describes the extent to which a specific Ada compiler conforms to the Ada Standard, ANSI/MIL-STD-1815A. This report explains all technical terms used within it and thoroughly reports the results of testing this compiler using the Ada Compiler Validation Capability. An Ada compiler must be implemented according to the Ada Standard, and any implementation-dependent features must conform to the requirements of the Ada Standard. The Ada Standard must be implemented in its entirety, and nothing can be implemented that is not in the Standard. Even though all validation Ada compilers conform to the Ada Standard, it must be understood that some differences do exist between implementations. The Ada Standard permits some implementation dependencies--for example, the maximum length of identifiers or the maximum values of integer types. Other differences between compilers result from the characteristics of particular operating systems, hardware, or implementation strategies. All the dependencies observed during the process of testing this compiler are given in this report. The information in this report is derived from the test results produced during validation testing. The validation process includes submitting a suite of standardized tests, the ACVC, as inputs to an Ada compiler and evaluating the results.

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AD-A242 273/1 PC A04/MF A01 National Inst. of Standards and Technology, Gaithers-

Add Compiler Validation Summary Report: Certificate Number: 910517S1.11164 U.S. Navy, AdaVAX, Version 5.0, (/OPTIMIZE), VAX11/785 (Host and Target).

Final rept 17 May 91, 72p

No software available for distribution.

Key..ords: \*Ada programming language, \*Compilers, Standardization, Test and evaluation, \*Validation summary reports, Computer program verification.

This Validation Summary Report describes the extent to which a specific Ada compiler conforms to the Ada Standard, ANSI/MIL-STD-1815A. This report explains all technical terms used within it and thoroughly reports the results of testing this compiler using the Ada Compiler Validation Capability. An Ada compiler must be implemented according to the Ada Standard, and any implementation-dependent features must conform to the requirements of the Ada Standard. The Ada Standard must be implemented in its entirety, and Standard must be implemented in its entirety, and nothing can be implemented that is not in the Standard. Even though all validation Ada compilers conform to the Ada Standard, it must be understood that some differences do exist between implementations. The Ada Standard permits some implementation dependencies--for example, the maximum length of identifiers or the maximum values of integer types. Other differences between compilers result from the characteristics of particular operating systems, hardware, or implementation strategies. All the dependencies observed during the process of testing this compiler are given in this report. The information in this report is derived from the test results produced during valida-tion testing. The validation process includes submitting a suite of standardized tests, the ACVC, as inputs to an Ada compiler and evaluating the results.

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AD-A242 609/6 PC A05/MF A01 National Inst. of Standards and Technology, Gaithersburg, MD.

Durg, MD.
Ada Compller Validation Summary Report: Certificate Number 910918S1.11216, NEC Corporation, NEC Ada Compller System for EWS-UX/V (Rel 4.0), Version Release 2.1(4.6) EWS4800/220 = EWS4800/220.

Final rept. 18 Sep 91, 77p No software available with this document.

Keywords: Standardization, Test and evaluation, \*Compilers, \*Ada programming language, \*Validation summary reports, Computer program verification.

This Validation Summary Report describes the extent to which a specific Ada compiler conforms to the Ada Standard, ANSI/MIL-STD-1815A. This report explains all technical terms used within it and thoroughly reports the results of testing this compiler using the Ada Compiler Validation Capability. An Ada compiler must be implemented according to the Ada Standard, and any implementation-dependent features must conform to the requirements of the Ada Standard. The Ada to the requirements of the Ada Standard. The Ada Standard must be implemented in its entirety, and nothing can be implemented that is not in the Standard. Even though all validated Ada compilers conform to the Ada Standard, it must be understood that some differences do exist between implementations. The Ada Standard permits some implementation dependencies--for example, the maximum length of identifiers or the maximum values of integer types. Other differences between compilers result from the characteris-tics of particular operating systems, hardware, or im-plementation strategies. All the dependencies observed during the process of testing this compiler are given in this report. The information in this report is derived from the test results produced during validation testing. The validation process includes submitting a suite of standardized tests, the ACVC, as inputs to an Ada compiler and evaluating the results.

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AD-A242 896/9 PC A04/MF AUI National Inst. of Standards and Technology, Gaithers-PC A04/MF A01 burg, MD.

Ada Compiler Validation Summary Report. Certificate Number: 911025S1.11226, Digital Equipment Corporation DEC Ada, Version 1.0 DECstation 5000 Model 200 => DECstation 5000 Model 200. Final rept. 28 Oct 91, 71p

Keywords: Standardization, Test and evaluation, \*Compilers, \*Ada programming language, \*Validation summary reports, Computer program verification.

This Validation Summary Report describes the extent to which a specific Ada compiler conforms to the Ada Standard, ANSI/MIL-STD-1815A. This report explains all technical terms used within it and thoroughly roports the results of testing this compiler using the Ada Compiler Validation Capability. An Ada compiler must be implemented according to the Ada Standard, and any implementation-dependent features must conform to the requirements of the Ada Standard. The Ada Standard must be implemented in its entirety, and nothing can be implemented that is not in the Standard. Even through all validated Ada compilers conform to the Ada Standard, it must be understood that some differences do exist between implementations. The Ada Standard permits some implementation dependencies--for example, the maximum length of identifiers or the maximum values of integer types. Other differences between compilers result from the characteristics of particular operating systems, hardware, or implementation strategies. All the dependencies observed during the process of testing this compiler are given in this report. The information in this report is derived from the test results produced during valida-tion testing. The validation process includes submitting a suite of standardized tests, the ACVC, as inputs to an Ada compiler and evaluating the results.

PC E09
National Inst. of Standards and Technology (CSL),
Gaithersburg, MD.
Graphical Kernel System (GKS). Pascal Binding; Software Standard; Subcategory: Graphics. Federal information processing standards (Final). Federal information processing standards (Final). D. R. Benigni. c1991, 179p Supersedes FIPS PUB 120. See also FIPS PUB 120-1 and FIPS PUB 120-1B. Also pub. as American National Standards Inst., New York rept. no. ANSI-X3.124.2-1988. Prepared in cooperation with American National Standards Inst., New York.

Three ring vinyl binder also available; North American Continent price \$7.00; all others write for quote.

Keywords: \*Computer graphics, \*Interactive graphics, Software, Requirements, Subroutines, Specifications, Federal Information Processing Standards Publications 120-1A, FIPS 120-1A, \*Graphical Kernel System, American National Standard Graphical Kernel System (ANSGKS) ANSI X3.124-1985, Language binding, Graphics software standard.

The revision supersedes FIPS PUB 120 and modifies the standard by adding a requirement for validation of GKS implementations that are acquired by Federal agencies. FIPS 120-1 adopts American National Standard Graphical Kernel System (ANS GKS), ANSI X3.124.1985, Functional Description, which consists for four parts (X3.124.1-1985 FORTRAN Binding, X3.124.2-1988 Pascal Binding, X3.124.3-1989 Ada Binding), as a FIPS. ANS GKS specifies a library (or toolbox package) of subroutines for an application programmer to incorporate within a program in order to produce and manipulate two-dimensional pictures. The purpose of the standard is to promote portability of graphics application programs between different installations. The standard is for use by implementors as the reference authority in developing graphics soft-ware systems; and by other computer professionals who need to know the precise syntactic and semantic rules of the standard.

100,637 PB91-134536 Not available NTIS
National Bureau of Standards (ICST), Gaithersburg,
MD. Systems and Software Technology Div.
Developing Federal Software Standards: A New Direction. Final rept. W. M. Osborne, and A. L. Hankinson. 1986, 2p

W. M. Osborne, and A. L. Hankinson. 1966, 2p Pub. in Proceedings of Computer Standards Confer-ence Striking a Balance between Technology, Eco-nomics, Politics, and Reality - for Substance, Not Form, San Francisco, CA., May 13-15, 1986, p1-2.

Keywords: Reprints, \*Federal information processing standards, \*Computer software, \*Software engineering, Software tools, Computer software maintenance, Computer program reliability, Computer software man-

The software community has made great strides in the application of engineering methods and tools to improve software quality and to enhance the productivity of the software development process. The discussion describes efforts underway at the National Institute of Standards and Technology to use software standards as a framework for developing, acquiring, and maintaining software during its operational life.

PB91-143289 PC A03/MF A01 National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Robot Systems Div.

Assembly Code to Compute Sine and Cosine Using the Cordic Algorithm.

J. A. Horst. Dec 90, 20p NISTIR-4480

Keywords: \*Computer calculations, Assembly languages, Algorithms, Computation, Computer programs, \*CORDIC algorithm, Sine, Cosine, Intel 8051 microcontrollers.

The CORDIC algorithm is commonly used to approximate certain elementary functions. Many microprocessor and microcontroller chips without the availability of math coprocessor chips could benefit from the effi-cient implementation of this algorithm. The focus of the work is to report on a specific implementation in assembly code (for an 8051 microcontroller) that computes the sine and cosine to eleven bits of accuracy.

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PB91-149179 Not available NTIS Mational Bureau of Standards (ICST), Gaithersburg, MD. Center for Computer Systems Engineering.

UNIX Expert: A Prototype Knowledge-Based Soft-

ware Development Workstation.

Final rept.

S. B. Salazar. 1985, 6p

Pub. in Intelligent Systems: Their Development and Application, p103-108 1985.

Keywords: \*UNIX(Operating system), \*Expert systems, Knowledge bases(Artificial intelligence), Software engineering, Workstations, Prototypes, Reprints.

U-Expert is a prototype expert system that assists in U-Expert is a prototype expert system that assists in resolving UNIX needs. Implementing this system has raised issues regarding the construction of complex knowledge-based systems, among them problems of organizing large amounts of knowledge and providing an acceptable interface for users of varying experience levels. These observations suggest that a programmer's assistant should combine artificial intelligence and policy levels. gence methods, such as rules, frames, and natural language processing, with more traditional approaches, such as graphics.

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PB91-149336 Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD

Algorithm Design for Large-Scale Computations.

Final rept. F. Sullivan. 1987, 7p

Pub. in International Jnl. of Supercomputer Applications 1, n1 p99-105 1987.

Keywords: \*Computer programming, Ising model, Supercomputers, Computation, Algorithms, Reprints, \*Algorithm design, Fractal dimensions, Molecular dynam-

Success in large scale scientific computations often depends on algorithm design. Even the fastest machine may prove to be inadequate unless sufficient attention is paid to the way in which the computation is organized. In the paper, the authors use several problems from computational physics to illustrate the importance of good algorithms, and they offer some very general principles for designing algorithms. Two subthemes are: first, the strong connection between the algorithm and the architecture of the target machine; and second, the importance of non-numerical methods in scientific computations.

100,641 PB91-157198

PC A07/MF A01

### **Computer Software**

National Inst. of Standards and Technology (NCSL),

Gaithersburg, MD.

Proceedings of the Object-Oriented Database
Task Group Workshop, Tuesday, October 23, 1990,
Chateau Laurier Hotel, Ottawa, Canada.

E. N. Fong. Jan 91, 150p NISTIR-4488

Keywords: \*Meetings, \*Data bases, \*Standardization, Data base management systems, Programming languages, Standards, Models, Data processing security, Query languages, \*Object-oriented programming.

The report constitutes the proceedings of a one-day workshop on standardization of object database systems. The workshop was the second attempt to solicit public input to identify what aspects of object database systems may be candidates for consensus that can lead to standards. The workshop goals focused on concrete proposals for languages or module inter-faces, exchange mechanisms, abstract specifications, common libraries, or benchmarks. The workshop announcement also solicited papers on relationships of object database systems capabilities to existing standards, including assertions that question the wisdom of standardization. The proceedings consist of 13 position papers covering various aspects where standardization on object database systems may be possible.

100,642

Not available NTIS PB91-159160 National Bureau of Standards, Gaithersburg, MD. Pro-

gram Office.
Agency Exploits Flexibility of Software in Moving Info.

Final rept. A. H. Sher, and P. B. Saunders. 1986, 1p. Pub. in Government Computer News 5, n9 p35(2), 9 May 86.

Keywords: \*Microcomputers, \*Computer software, \*Data bases, Word processing, Data conversion, Data base management systems, Text processing, Data dictionaries, Reprints.

The article examines problems encountered when data is not in a form immediately suitable for a particular software package. It describes two applications. In the first, global word processor commands are used to convert text files created on a variety of hardware and software systems to a format that can be imported directly into a database file; in the second, the use of database management software enhances the utility of a directory by permitting queries on any information field or part thereof without restricting searches to a rigid list of prespecified keywords.

100,643

PB91-159723 PC A14/MF A02 National Inst. of Standards and Technology (NCSL),

National Inst. of Standards and Technology (NCSL), Gaithersburg, MD.

Proceedings of the Object-Oriented Database Task Group Workshop. Held in Atlantic City, New Jersey on May 22, 1990. E. N. Fong, and C. W. Thompson. Feb 91, 308p NISTIR-4503

See also PB91-157198. Prepared in cooperation with Texas Instruments, Inc., Dallas.

Keywords: \*Meetings, \*Data bases, \*Standardization, Data base management systems, Programming languages, Standards, Models, Information systems, Query languages, \*Object-oriented programming.

The report constitutes the proceedings of a one-day workshop on standardization of object database sys-tems. The workshop was the first of two workshops held to solicit public input to identify what aspects of object database systems may be candidates for con-sensus that can lead to standards. The workshop attempted to focus on concrete proposals for language or module interfaces, exchange mechanisms, abstract specifications, common libraries, or benchmarks. The workshop announcement also solicited papers on the relationship of object database system capabilities to existing standards, including assertions that question the wisdom of standardization. The proceedings consists of 22 position papers covering various aspects where standardization on object database systems may be possible.

100,644

PB91-167387 PC A04/MF A01 National Inst. of Standards and Technology (NCSL), Gaithersburg, MD.

Functional Benchmarks for Fourth Generation Languages.

Special pub. (Final) M. M. Gray, and G. E. Fisher. Mar 91, 61p NIST/SP-500/184

Also available from Supt. of Docs. as SN003-003-03071-6. See also PB87-210332.

Keywords: \*Tests, Data base management, High level languages, Methodology, Man computer interface, Computer graphics, Data processing security, Software engineering, Application programs(Computers), \*Fourth generation languages, \*Functional bench-

In recent years, fourth generation language (4GL) usage has expanded in data processing organizations, especially where end-users have assumed increased programming responsibilities. Since there are no 4GL standards, managers selecting a 4GL need some method of determining how well a particular 4GL will meet organizational, application, and user requirements. The report provides a methodology to assist in that determination. It contains 'functional benchmarks' (as opposed to performance benchmarks) consisting of a testing methodology and descriptions of tests to evaluate the capabilities of a particular 4GL in relation to organizational requirements. Test results are evaluated at two levels: the 4GL's ability to perform a task, and the ease of performing it. These evaluations are combined with user-defined weighted requirements to produce an overall rating for each 4GL tested.

100,645

PB91-174441 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Applied and Computational Mathematics Div.

DEQSOL and ELLPACK: Problem-Solving Environments for Partial Differential Equations.

Final rept. R. F. Boisvert, and D. K. Kahaner. 1991, 13p Pub. in Office of Naval Research Asian Office Scientific Information Bulletin 16, n1 p7-19 Jan/Mar 91.

Keywords: \*Partial differential equations, \*Computer programming, Elliptic differential equations, Boundary value problems, Numerical integration, Supercomputers, Fortran, Reprints, DEQSOL system, ELLPACK

A number of integrated problem-solving environments for the solution of partial differential equations have been developed in recent years. Such systems permit very-high-level descriptions of the mathematical problem and its solution algorithm. These descriptions are translated into efficient Fortran programs that produce solutions in both tabular and graphical forms. In the paper the authors compare and contrast two such systems: DEOSOL, a Japanese project, and ELLPACK, an American project. For each system, the authors present a brief history, describe its capabilities, and present several examples of its use.

100.646

PB91-175455 Not available NTIS National Bureau of Standards (ICST), Gaithersburg, MD. Information Systems Engineering Div. Designing Data Entity Naming Conventions.

J. Newton. 1988, 11p Pub. in Proceedings of International Conference on Entity-Relationship Approach (6th), New York, NY., November 9-11, 1987, p439-449 1988.

Keywords: \*Data bases, \*Data management, Data base administrators, Data dictionaries, Standards, Data structures, Reprints, Information Resource Dictionary System.

A coherent set of naming conventions for data entities is crucial to the central management of data. Name content and format must be designed to maximize the information content and relationship to the logical structure of the data. Information Resource Dictionary System (IRDS) metaname structure provides a frame-work for name development; a methodology is de-scribed for mapping between an entity's data dictionary names.

100 647

PB91-185108 PC A04/MF A01 National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Applied and Computational MatheVolksGrapher: a FORTRAN Plotting Package User's Guide, Version 3.0.
D. K. Kahaner, and W. E. Anderson. Feb 90, 55p NISTIR-90/4238

Keywords: \*Plotting, \*Subroutines, Fortran programming language, Two dimensional, Interactive systems, Printers(Data processing), User manuals(Computer programs), VolksGrapher computer program.

VolksGrapher(VG) is a collection of FORTRAN callable subroutines for plotting two dimensional data. The main features of VG are: Portability; Ease of use; Realistic flexibility; Built-in interactivity; Support for several printers; Works in the window environment of the Sun; VG is in the public domain.

100.648 PB91-187567 PC A04/MF A01 National Inst. of Standards and Technology (CSL),

Gaithersburg, MD.

Guide to Design, Implementation and Management of Distributed Databases.

Special pub. E. N. Fong, C. L. Sheppard, and K. A. Harvill. Feb 91, 60p NIST/SP-500/185

Also available from Supt. of Docs. as SN003-003-

Keywords: \*Data base management systems, \*Distributed computer systems, Data bases, Life cycles, Computer systems hardware, Computer systems programs, Systems engineering, Computer networks, Computer communications, Computer software, Data dictionaries, Protocols.

For an organization to operate in a distributed database environment, there are two related but distinct tasks that must be accomplished. First, the distributed database environment must be established. Then, a distributed database application can be designed and installed within the environment. The guide describes both of these activities based on a development life-cycle phase framework. The guide provides practical information and identifies skills needed for systems designers, application developers, database and data administrators who are interested in the effective planning, design, installation, and support for a distributed database environment. In addition, the guide instructs system analysts and application developers with a step-by-step procedure for the design, implementation and management of a distributed data base management system (DBMS) application. The guide also notes that truly heterogeneous distributed database technology is still a research consideration.

100.649 PB91-187716 PC A04/MF A01 National Inst. of Standards and Technology (NCSL), Gaithersburg. MD. Software Standards Validation Gaithersburg, MD. Software Standards

Group.
Programming Languages and Database Language SQL. Validated Processor List Including GOSIP Conformance Testing Registers.
J. B. Kailey. Apr 91, 59p NISTIR-4557

Keywords: \*Compilers, \*Operating systems(Computers), \*Validity, Federal information processing standards, PASCAL programming language, Query languages, Tests, Data bases, Ada programming language, COBOL programming language, Fortran programming language, SQL programming language, Federal Information Resources Management Deculotions ment Regulation.

The Validated Processor List identifies those COBOL. Fortran, Ada, and Pascal programming language processors that have a current validation certificate and essors that have a current validation certificate and those SQL language processors that have a registered test report, referencing the applicable Federal Information Processing Standard (FIPS) as of the date of the publication. The testing of language processors to determine the degree to which they conform to the Federal Standards is required by Government agencies as specified by the FIPS, Federal Information Resources Management Regulation (FIRMR) Parts 201.13 and 201.39, and the associated Federal ADP and Telecommunications Standards Index. The List is and Telecommunications Standards Index. The List is updated and published quarterly.

100.650

PB91-189456 Not available NTIS National Inst. of Standards and Technology (NCSL), Gaithersburg, MD. Systems and Software Technology

**Computer Software** 

Difficulties in Parsing SGML.

Final rept. J. Heath, and L. Welsch. 1988, 7p

Pub. in Proceedings of ACM Conference on Document Processing Systems, Santa Fe, NM., December 5-9, 1988, p71-77.

Keywords: \*Parsers, Documents, Parsing algorithms, Reprints, Programming languages, Translators, Repr \*SGML(Standard Generalized Markup Language).

A frequently cited problem with the Standard Generalized Markup Language (SGML) is that applications using the standard have been slow in arriving. Part of this delay is because of the instability of the standard and part because of constructs of the language that are functionally redundant and/or add unnecessary complexity to both machine and human processing. The paper examines the implementation of an SGML parser using commonly available tools for building programming language translators. It describes the prob-lems encountered and suggests modifications to SGML to eliminate those problems. The modified language can be implemented using well tested tools and will be more stable and more amenable to both computer and human processing while maintaining all of the fundamental strengths of SGML.

100,651

PB91-201772 PC A03/MF A01 National Inst. of Standards and Technology (NCSL), Gaithersburg, MD. Software Standards Validation

FORTRAN Temporary Program Fixes, FCVS78 Version 2.0, Level 26. 1 Feb 87, 22p

See also PB85-226736 and PB82-250903.

Keywords: \*Compilers, \*Error correction codes, Errors, Tests, Computer program verification, Comput-er software maintenance, Debugging(Computers), er software maintenance, 2. \*Fortran programming language.

The report is a supplement to the 1978 FORTRAN Compiler Validation System (FCVS78) User's Guide which documents the errors that are contained in Version 2.0 of the FCVS78. An update to the FCVS78 is referred to as Temporary Program Fix (TPF). These TPF's must be applied to the FCVS78 population tape to correct the identified errors and will be used in conducting an official validation. An explanation of each error is provided in the 'description of problem' paragraph together with the name of the test(s), if any, affected by the error.

100.652 PB91-216598 PC A03/MF A01 National Inst. of Standards and Technology (CAML), Gaithersburg, MD.

Portable Vectorized Software for Bessel Function Evaluation.

Boisvert, and B. V. Saunders. Jun 91, 18p R. F. Boisvert NISTIR-4615

Keywords: \*Bessel functions, \*Computer programming, Vector processing, CRAY computers, Computation, Algorithms, Fortran 77 programming language, Chebyshev series, Portability, VFNLIB system.

A suite of computer programs for the evaluation of Bessel functions and modified Bessel functions of Bessel functions and modified Bessel functions of orders zero and one for a vector of real arguments is described. Distinguishing characteristics of these programs are that (1) they are portable across a wide range of machines, and (2) they are vectorized in the case when multiple function evaluations are to be performed. The performance of the new programs are compared with software from the FNLIB collection of Fullation on which the new software is based. Fullerton on which the new software is based.

100.653

PB91-222588 PC A03/MF A01 National Inst. of Standards and Technology (CSL), Gaithersburg, MD. Advanced Systems Div.

Performance Evaluation of Hypercube Applications: Using a Global Clock and Time Dilation.

R. D. Snelick. Jul 91, 27p NISTIR-4630
Sponsored by Defense Advanced Research Projects Agency, Arlington, VA., and Department of Energy, Washington, DC.

Keywords: \*Hypercube multiprocessors, Parallel processing, Performance evaluation, Time dilation.

Time dilation provides an accurate method for investigating the performance of an application using a varie-

ty of physical transport speeds. Measuring sources of communication delay in a global domain reveals performance data that are important in the analysis of loosely-coupled machine applications. Together, time dilation and communication delay measurement provide an environment that offers insight for the development and analysis of concurrent algorithms and architectures. Logical and physical transport latencies indi-cate whether a poorly performing application needs a new algorithm (less logical delay) or a faster interconnection hardware (less physical delay). Other algorithmic and architectural characteristics are revealed with the performance evaluation measurements. The runtime statistics should be available to programmers so that necessary steps can be taken to improve their programs.

100,654 PB91-231571 PC A03/MF A01 National Inst. of Standards and Technology (CSL), Gaithersburg, MD. Database and Graphics Group. Computer Implementation of a Discrete Set Alge-

L. Gallagher. Jul 91, 31p NISTIR-4637

Keywords: \*Data management, \*Set theory. Trees(Mathematics), Data structures, Boolean algebra, Algorithms, Binary trees.

Large finite sets occur naturally in computer data management. Discrete elements such as numbers, pointers, icons, and object identifiers all have fixed-length bit sequence representations that may be viewed as base-two integers. The efficiencet storage and manipulation of large collections of such items is a long-standing problem in computer science. In particular, many data management algorithms may be specified in terms of set operations (e.g. union, intersection, crossproduct) on these collections. Often a large set is stored in reduced form for storage efficiency. A specific problem is then to find efficient algorithms for per-forming set operations over the reduced representations. The paper presents a binary tree storage mechanism for efficient representation of arbitrary sets of discrete elements taken from a fixed universe. It then develops high-level algorithms for mapping these sets to and from their tree representations and for executing set operations directly on the storage representa-tion itself. This approach provides a method for direct computer implementation of mathematical models based on Boolean algebras defined over finite sets.

100 655

PB91-236687 Not available NTIS National Inst. of Standards and Technology (CSL), Gaithersburg, MD. Systems and Software Technology

Functional Meta-Structure for Hypertext Models and Systems. Final rept.

R. Furuta, and P. D. Stotts. 1990, 27p Pub. in Electronic Publishing 3, n4 p179-205 Nov 90.

Keywords: \*Models, Systems analysis, Publishing, Information retrieval, Reprints, \*Hypertext, Meta-struc-

The authors describe a hypertext 'meta-structure'-one that provides an organization for the architecture of hypertext models and systems. The meta-structure was initially developed to help us understand the architecture of a specific hypertext model (the Trellis hypertext model). However, its organization seems generally applicable to a wide range of other models and systems as well. As such, the meta-structure is a good candidate for a high-level hypertext reference model, and so they refer to it as the Trellis hypertext reference model, or the r-model. The r-model represents a hypertext at five levels of abstraction-two abstract levels, two concrete levels, and one visible level. In the paper, they present the r-model, use it to classify four different hypertext (and hypertext-like) systems, and then discuss its relationship to various hypertext-defined concepts.

PB91-237040 Not available NTIS National Inst. of Standards and Technology (CSL), Gaithersburg, MD. Systems and Software Technology

Book Review: Hypertext Hands-On.

Final rept. J. Moline. 1990, 2p Pub. in Electronic Publishing 3, n3 p173-174 Aug 90.

Keywords: \*Books, \*Reviews, Information retrieval, Publishing, Computer software, Systems engineering, Reprints, \*Hypertext.

Hypertext Hands-On, by Ben Shneiderman and Greg Kearsley, is an excellent introduction to hypertext, whether in book or electronic form. The serious user of the material should start with the software. It provides a quick introduction to this new way of organizing and accessing information through examples of potential hypertext applications that could not be represented in the book. These applications provide a context for the concepts of hypertext. The authors have included material on how hypertext works, why one might use it, things of concern to system designers, and help on authoring and implementing a hypertext. Further, they have included a discussion of many of the commercial hypertext systems and also articles on the major personalities in the development of the hypertext concept. The book, whether as a hyperbook or a hardback, is an excellent introduction to this new approach of organizing and accessing information.

100,657

Not available NTIS PB91-237057 National Inst. of Standards and Technology (CSL), Gaithersburg, MD. Systems and Software Technology

Linking Information to Objects: A Hypertext Prototype for Numismatists.

Final rept.

J. Moline. 1991, 17p

Pub. in Visual Resources VII, p361-377 1991.

Keywords: \*Museums, \*Information systems, Computer applications, Prototypes, Data bases, Man computer interface, Parallel processing, Reprints, \*Numismatics, \*Hypertext.

The researcher discusses a hypertext prototype developed to provide for the information needs of numismatists, particularly those working with early Arab coins The structure of the prototype is discussed showing the organization of the information bases, the links among information bases, and the links to tools which facilitate the work of the researcher. The information bases include image bases, object bases, and docu-ment bases. Hypertext provides a user interface with simple links to allow non-sequential browsing of the material, as well as complex links which integrate other components into the prototype. The purpose of the paper to present a system of limited scope as a basis for discussing how it deals with some of the issues which may be important in museum settings. It is expected that this research could serve as a model for the development of parallel systems for other user groups. Further, it is expected that this prototype will provide a better understanding of the technologies available and their role in facilitating information use by a particular user community.

100.658

PB91-237685 Not available NTIS National Inst. of Standards and Technology (CSL), Gaithersburg, MD. Systems and Software Technology

Software Verification and Validation: An Overview. Final rept.

D. R. Wallace, and R. U. Fujii. 1989, 8p

See also PB90-111691.
Pub. in IEEE (Institute of Electrical and Electronics Engineers) Software 6, n3 p10-17 May 89.

Keywords: \*Computer program verification, \*Software engineering, \*Computer software management, Standards, Guidelines, Computer software maintenance, Tests, Reprints.

The application of software verification and validation (V&V) to the development and maintenance of computer software is governed by three types of software puter software is governed by three types of software engineering standards and guidelines: those identifying requirements for planning and performing software V&V, those requiring software V&V, and those including software V&V activities as part of their domain. Specific definitions, requirements, and approaches vary among them but together they provide strong discould be a software variety and improvements. rection for planning and implementing a software verification and validation effort which includes software testing.

100,659

PB91-240754 PC A03/MF A01 National Inst. of Standards and Technology (MEL), Gaithersburg, MD. Robot Systems Div.

# Computer Software

Depot: A Framework for Sharing Software Installation Across Organizational and Unix Platform

K. L. Manheimer, S. N. Clark, B. A. Warsaw, and W. P. Rowe. Sep 90, 14p NISTIR-4436

Prepared in cooperation with Century Computing, Inc.,

Keywords: \*Distributed computer systems, \*Computer software, \*Installing, UNIX(Operating system), File management systems, Distributed processing, USR local.

The depot provides a coherent and accomodating framework for distributing and administering nonstandard UNIX applications across extensibly numerous and diverse computer platforms. It is designed to promote sharing of expertise and disk resources necessary to maintain elaborate third-party applications, supplementing the utility of ad hoc /usr/local arrangement in a formal scheme that allows extension across non-homogeneous clusters of hosts. In particular, it facilitates software installation, release, and accomodation across multiple platforms and diverse host configurations. The authors have implemented the Depot using conventional UNIX subsystems and resources com-bined with policies for coordinating them. The paper presents the specific aims, structure, and rationale of the depot framework in sufficient detail to facilitate its implementation elsewhere.

100.660 PB91-507699 CP T99
MUMPS System Lab., Nagoya (Japan).
MUMPS Validation Suite, Version 7.6 (Vax/VMS

Backup), 1991.

1 Mar 91, mag tape NIST/SW/MT-91/011 System: DEC PDP-11/34; Vax/VMS Version V5.3 operating system. Language: MUMPS. File format: Vax/ VMS Backup. Other formats available as PB91-507707 (for Microcomputers), PB91-507715 (ANSI), and PB91-507723 (TAR). Sponsored by National Inst. of Standards and Technology, Gaithersburg, MD. Available in 9-track, ASCII character set, 1600 or 6250

Keywords: \*Software, \*Compilers, \*Tests, Federal information processing standards, Precompilers, Validation summary reports, Computer systems programs, Computer program verification, Interpreters, Magnetic tapes, \*MUMPS programming language.

Version 7.6 of the ANSI/MDC X11.1-1984 MUMPS Validation Suite (the MVS) is the revision of Version 7.51 (August, 1990) designed to meet the requirements in FIPS PUB 125 for a conformance test method. The revision was made with U.S. reviewers' comments and suggestions in order to incorporate into the validation suite such features as computer detection of integrity of the validation suite, pass/fail conditions of individual tests, checkpointing test runs to enable interrupted test process to restart from the most suitable position, instructions and warnings at adequate points, and fully automated tabulation of the Validation Summary Report (the VSR). Provision of such features will facilitate evaluation of the validation process by relegating these time-consuming tasks to the computer, assisted by a few experienced personnel.

100,661 PB91-507707 **CP D99** MUMPS System Lab., Nagoya (Japan). MUMPS Validation Suite, Version 7.6, 1991 (for

Microcomputers). Software.

1 Mar 91, 2 diskettes NIST/SW/DK-91/012 System: IBM PC/XT; MS DOS 3.0 or higher operating system. Language: MUMPS. Supersedes PB90-500125. Other formats available as PB91-507699 (Vax/VMS), PB91-507715 (ANSI), and PB91-507723 (TAR). Sponsored by National Inst. of Standards and Technology, Gaithersburg, MD. The software is on two 1.2M, 5.1/4 inch diskettes, high

density. The diskettes are in ASCII format.

Keywords: \*Software, \*Compilers, \*Tests, Microcomputers, Federal information processing standards, Precompilers, Validation summary reports, Computer systems programs, Computer program verification, Interpreters, Diskettes, \*MUMPS programming language.

Version 7.6 of the ANSI/MDC X11.1-1984 MUMPS Validation Suite (the MVS) is the revision of Version 7.51 (August, 1990) designed to meet the require-

ments in FIPS PUB 125 for a conformance test method. The revision was made with U.S. reviewers' comments and suggestions in order to incorporate into the validation suite such features as computer detection of integrity of the validation suite, pass/fail conditions of individual tests, checkpointing test runs to enable interrupted test process to restart from the most suitable position, instructions and warnings at adequate points, and fully automated tabulation of the Validation Summary Report (the VSR). Provision of such features will facilitate evaluation of the validation process by relegating these time-consuming tasks to the computer, assisted by a few experienced person-

100.662 PB91-507715 CP T99 MUMPS System Lab., Nagoya (Japan). MUMPS Validation Suite, Version 7.6 (ANSI), 1991. Software

Software.

1 Mar 91, mag tape NIST/SW/MT-91/013

System: DEC PDP-11/34. Language: MUMPS. Supersedes PB90-500117. Other formats available as PB91-507699 (Vax/VMS Backup), PB91-507707 (for Microcomputers), and PB91-507723 (TAR). Sponsored by National Inst. of Standards and Technology, Gaithersburg MD. burg, MD.

Available in 9-track, ASCII character set, 1600 or 6250

Keywords: \*Software, \*Compilers, \*Tests, Federal information processing standards, Precompilers, Validation summary reports, Computer systems programs, Computer program verification, Interpreters, Magnetic tapes, \*MUMPS programming language.

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100 663 PB91-507723 CP T99 MUMPS System Lab., Nagoya (Japan). MUMPS Validation Suite, Version 7.6 (TAR), 1991.

Software.

1 Mar 91, mag tape NIST/SW/MT-91/014

System: DEC PDP-11/34; VAX/VMS Version V5.3 operating system. Language: MUMPS. Other formats available as PB91-507699 (Vax/VMS Backup), PB91-507707 (for Microcomputers), and PB91-507715 (ANSI). Sponsored by National Inst. of Standards and Technology Gaithershurg, MD. Technology, Gaithersburg, MD. Available in 9-track, ASCII character set, 1600 or 6250

Keywords: \*Software, \*Compilers, \*Tests, Federal information processing standards, Precompilers, Validation summary reports, Computer systems programs, Computer program verification, Interpreters, Magnetic tapes, \*MUMPS programming language.

Version 7.6 of the ANSI/MDC X11.1-1984 MUMPS Validation Suite (the MVS) is the revision of Version 7.51 (August, 1990) designed to meet the requirements in FIPS PUB 125 for a conformance test method. The revision was made with U.S. reviewers' comments and suggestions in order to incorporate into the validation suite such features as computer detection of integrity of the validation suite, pass/fail conditions of individual tests, checkpointing test runs to enable interrupted test process to restart from the most suitable position, instructions and warnings at adequate points, and fully automated tabulation of the Validation Summary Report (the VSR). Provision of such features will facilitate evaluation of the validation process by relegating these time-consuming tasks to the computer, assisted by a few experienced person-

100,664 PB91-937301 Not available NTIS National Inst. of Standards and Technology, GaithersValidated Processor List (Cobol, Fortran, ADA, Pascai, SQL). July 1991. Jul 91, 65p NISTIR/4623

Keywords: Cobol Programming Language, Fortran Programming Language, Language Programming.

Validated Processor List identifies those COBOL, Fortran, ADA and Pascal programming language processors that have a current validation certificate and those SQL language processors that have a registered test report, referencing the applicable Federal Information Processing Standard (FIPS) as of the date of this publication. This list also includes GOSIP Conformance Testing Registers. The testing of language processors to determine the degree to which they conform to the Federal Standards is required by Government agencies in accordance with Federal Information Resources Management Regulation (FIRMR) Parts 201.13 and 201.39, and the associated Federal ADP and Telecommunications Standards Index. The list is updated and published quarterly.

100,665 PB91-937302 Not available NTIS National Inst. of Standards and Technology, Gaithers-Validated Processor List (Cobol, Fortran, ADA, Pascal, SQL). October 1991. Oct 91, 94p NISTIR/4690 Supersedes PB91-937301.

Keywords: Cobol Programming Language, Fortran Programming Language, Language Programming.

Validated Processor List identifies those COBOL, Fortran, ADA and Pascal programming language processors that have a current validation certificate and those SQL language processors that have a registered test report, referencing the applicable Federal Information Processing Standard (FIPS) as of the date of this publi-cation. This list also includes GOSIP Conformance Testing Registers. The testing of language processors to determine the degree to which they conform to the Federal Standards is required by Government agencies in accordance with Federal Information Resources Management Regulation (FIRMR) Parts 201.13 and 201.39, and the associated Federal ADP and Telecommunications Standards Index. The list is updated and published quarterly.

PC A07/MF A02 PB92-108943 National Inst. of Standards and Technology (CSL), Gaithersburg, MD. Development of an Optical Disk System for the Automated Retrieval of EASEAR Records.

Final rept. N. Willman. Aug 91, 139p NISTIR-4654

Sponsored by Social Security Administration, Baltimore, MD.

Keywords: \*Information retrieval, \*Optical disks, Programming manuals, Computer programs, Magnetooptics, Automation, Feasibility, Pilot studies, \*Social Security Administration, EASEAR pilot system, EASEAR

The Social Security Administration (SSA) maintains records of the yearly wages earned by every person in the United States. Each year, approximately 2.5 giga-bytes of data are collected on self-employed wage earners, and 47 gigabytes of data are collected on other wage earners. The records are currently stored on over 110,000 rolls of microfilm. It takes over 400 scouts to retrieve information needed by the professional staff. Often, the needed roll of film is missing from the file due to being currently in use, misfiled, or misplaced. In addition, the information obtained from the microfilm is not always the most current, and decisions are sometimes based on obsolete data. Advances in peripheral mass storage technology during the 1980s (e.g. magneto-optic recording) now allow for alternate approaches to data storage and retrieval. It is believed that an automated retrieval system would provide a more accurate, timely, and cost effective means of retrieving information. The pilot application detailed in the document is intended to demonstrate the feasibility of a full scale automated records retrieval system, to study the impact of an automated system on the users, and to gain insight into the factors which would impact the design of a full scale system.

100,667 PB92-109040

PC A03/MF A01

### Computer Software

National Inst. of Standards and Technology (CSL),

Gaithersburg, MD.

Proceedings of the Workshop on High Integrity
Software. Held in Gaithersburg, MD. on January 22-23, 1991.

22-23, 1991.
Special pub. (Final).
D. R. Wallace, D. R. Kuhn, and J. C. Cherniavsky.
Aug 91, 11p NIST/SP-500/190
Also available from Supt. of Docs. as SN003-00303108-9. Prepared in cooperation with National Science Foundation, Washington, DC.

Keywords: \*Meetings, \*Computer program reliability, \*Computer software, \*Standards, Standardization, Computer security, Benefit cost analysis, Safety, Data integrity, Computer software management, Hazards, Criticality, \*NIST.

The paper provides information related to the National Institute of Standards and Technology (NIST) effort to coordinate an effort to produce a comprehensive set of standards and guidelines for the assurance of high integrity software. The effort may include adapting or adopting existing standards as appropriate. In particular, the paper presents the results of a Workshop on the Assurance of High Integrity Software held at NIST on January 22-23, 1991. Workshop participants ad-dressed techniques, costs and benefits of assurance, controlled and encouraged practices, and hazard analysis. A preliminary set of recommendations was pre-pared and future directions for NIST activities in this area were proposed.

100,668 PB92-112267 PC A04/MF A01 National Inst. of Standards and Technology (CSL),

Gaithersburg, MD.

Proceedings of the Forum on Standards for High Integrity Software (DOD, Government, Industry). Held in Gaithersburg, Maryland on June 28, 1991. D. R. Wallace, M. Brown, and A. McKinlay. Sep 91,

64p NISTIR-4656 See also PB92-109040. Prepared in cooperation with Naval Surface Warfare Center, Dahlgren, VA., and McDonnell Douglas Corp., St. Louis, MO.

Keywords: \*Meetings, \*Computer software, \*Computer security, \*Standards, Quality assurance, Safety, Software engineering, Hazards, Computer program reliability, Computer program verification.

The report provides information related to the Forum on Standards for High Integrity Software (Department of Defense, Government, and Industry) held at the National Institute of Standards and Technology (NIST) on June 28, 1991. At the forum, software engineering ex-perts presented their perspectives on the role of soft-ware engineers in software safety, a comparison for safety and computer security issues in standards, hazard analysis, assurance standards, and software certification. Future directions for NIST activities for assurance of high integrity software were proposed.

100,669 PB92-116417 PC A03/MF A01 National Inst. of Standards and Technology (CSL), Gaithersburg, MD.

Software Reengineering: A Case Study and Lessons Learned.

Special pub. (Final). M. K. Ruhl, and M. T. Gunn. Sep 91, 42p NIST/SP-500/193

Also available from Supt. of Docs. as SN003-003-03100-3. See also N91-24047.

Keywords: \*Software engineering, Computer software maintenance, Case studies, Cost effectiveness, Recommendations, \*Software reuse, CASE(Computer Aided Software Engineering).

The report is aimed at managers and technical personnel (both Federal Government and industry) who need to understand: the concepts and issues of software reengineering; the use of Computer Aided Software Engineering (CASE) tools in the reengineering process; and the application of the technology to organizational problems. Software reengineering involves the use of existing software and documentation to specify requirements, design, documentation, and to produce software for a target platform. CASE tools are expected to play an important role in automating parts of the reengineering process. In the report software reengin-eering and other related terms are defined and possible benefits that relate to the technology are de-scribed. The use of CASE tools for reengineering are examined. A case study that examines the feasibility and cost-effectiveness of software reengineering is described. Study results are addressed along with recommendations for organizations that are considering the use of reengineering.

100,670

PB92-117308 Not available NTIS National Inst. of Standards and Technology (NCSL), Gaithersburg, MD. Systems and Software Technology

Interactive Video Software Portability: Migrating a DOS Application to POSIX.

Final rept.

R. D. Schneeman. 1991, 9p

Pub. in Proceedings of the Annual Technical Symposium (29th) Advanced Information Interfaces: Making Data Accessible, Washington, DC., June 19-20, 1991,

Keywords: \*Computer program portability, \*Disk operating system(DOS), Video disks, Interactive systems, Computer program transferability, Computer software, Interruption, Computer graphics, Reprints, \*POSIX(Portable Operating System Interface for Computer Environments).

Research on the migration of an MS-DOS based Interactive Video (IV) application to the Portable Operating System Interface for Computer Environments (POSIX) has revealed several key portability concerns. Namely, when (1) mapping the MS-DOS software interrupt application interface into a suitable POSIX paradigm; (2) implementing the necessary subset of IV commands from the Interactive Mulitmedia Association's (IMA), Recommended Practices for Multimedia Portability document; and (3) supplanting the original graphics capabilities with an Open Systems windowing solution. The paper addresses the above concerns in the context of migrating an MS-DOS application into a POSIX environment. The computing environment used in the research study and the target application are described fully.

100.671

PB92-937300 Standing Order National Inst. of Standards and Technology, Gaithersburg, MD.

Validated Products List (Cobol, Fortran, ADA, Pascal, MUMPS, SQL).

1992, 1p

Supersedes PB91-937300.

Paper copy available on Standing Order, deposit account required (U.S., Canada, and Mexico \$100; all others \$200). Single copies also available in paper copy only.

Keywords: \*Cobol programming language, \*Fortran regramming language, Fortian programming language, Fortian Federal Information Processing Standards, \*Validation summary reports, \*Pascal programming language, \*Ada programming language, SQL programming language, \*Ada programming language, SQL programming language, \*Ada programming language, SQL programming language, \*Ada programming language, quage.

The Validated Processor List identifies those COBOL, Fortran, Ada and Pascal programming language processors that have a current validation certificate and essors that have a current validation certificate and those SQL language processors that have a registered test report, referencing the applicable Federal Information processing Standard (FIPS) as of the date of the publication. The list also includes GOSIP Conformance Testing Registers. The testing of language processing Registers. essors to determine the degree to which they conform to the Federal Standards is required by Government agencies in accordance with Federal Information Resources Management regulation (FIRMR) Parts 201.13 and 201.39, and the associated Federal ADP and Telecommunications Standards Index. The list is updated and published quarterly.

### Information Processing Standards

100.672

FIPS PUB 100-1 PC A03 National Inst. of Standards and Technology (NCSL), Gaithersburg, MD. PC A03 Interface between Data Terminal Equipment (DTE) and Data Circuit-Terminating Equipment (DCE) for Operation with Packet-Switched Data Networks (PSDN), or between Two DTEs, by Dedicated Circuit. Category: Hardware Standard. Subcategory: Data Transmission.

Final rept.

c1989, 24p

Also pub. as American National Standards Inst., New York rept. no. ANSI-X3.100-1989. Supersedes FIPS PUB 100. Prepared in cooperation with American Na-tional Standards Inst., New York.

Three ring vinyl binder also available; North American Continent price \$7.00; all others write for quote.

Keywords: \*Computer networks, \*Data processing terminals, Telecommunication, \*Interfaces, \*Federal Information Processing Standards, \*Communication networks, Communication terminals, X-25 protocol, Packet switching.

The Federal Information Processing Standard (FIPS) specifies the interface between data terminating equipment (DTE) such as automated data processing (ADP) equipment and telecommunication system terminal equipment, and data circuit-terminating equipment (DCE) for operation in the packet mode on packet-switched data networks (PSDN), or between two DTEs, by dedicated circuit. The revised standard adopts American National Standard ANSI X3.100-1989 which in turn adopts CCITT Recommendation X-25-1988 developed by the Consultative Committee on International Telephone and Telegraph, and ISO 7776-1986 and ISO 8208-1987 developed by the International Organization for Standardization. The revision supersedes FIPS 100/FED-STD 1041. More detailed specifications on the applicable interface points for the standard in an Integrated Services Digital Network (ISDN) environment will be developed for a future FIPS for ISDN.

100.673

PC E15
National Inst. of Standards and Technology (CSL),
Gaithersburg, MD.
Graphical Kernel System (GKS); Category: Soft-

Graphical Kernel System (GRS); Category: Software Standard; Subcategory: Graphics.
Federal information processing standards (Final).
D. R. Benigni. c1991, 401p
Supersedes FIPS PUB 120. See also FIPS PUB 120-1A and FIPS PUB 120-1B. Also pub. as American National Standards Inst., New York rept. no. ANSI-X3.124-1985. Prepared in cooperation with American National Standards Inst. New York National Standards Inst., New York.

Three ring vinyl binder also available; North American Continent price \$7.00; all others write for quote.

Keywords: \*Computer software, \*Federal information processing standards, Computer graphics, Fortran, Pascal programming language, Validation, Ada programming language, \*Graphic Kernel System, Language, \*Graphic guage binding.

The report's revision supersedes FIPS PUB 120 and modifies the standard by adding a requirement for validation of GKS implementations that are acquired by Federal agencies. FIPS 120-1 adopts American National Standard Graphical Kernel System (ANS GKS), ANSI X3.124-1985, Functional Description, which consists of four parts (X3.124.1-1985 FORTRAN Binding, X3.124.2-1988 Pascal Binding, X3.124.3-1989 Ada Binding), as a FIPS. ANS GKS specifies a library (or toolbox package) of subroutines for an application programmer to incorporate within a program in order to produce and manipulate two-dimensional pictures. The purpose of the standard is to promote portability of graphics application programs between different installations. The standard is for use by implementors as the reference authority in developing graphics soft-ware systems; and by other computer professionals who need to know the precise syntactic and semantic rules of the standard.

100,674

**FIPS PUB 120-1B** National Inst. of Standards and Technology (CSL), Gaithersburg, MD. Graphical Kernel System (GKS). Ada Binding; Cat-

egory: Software Standard; Subcategory: Graphics.

Federal information processing standards (Final).
D. R. Benigni, c1991, 218p
Supersedes FIPS PUB 120. See also FIPS PUB 120-1
and FIPS PUB 120-1A. Also pub. as American National
Standards Inst., New York rept. no. ANSI-X3.124.3-

### Information Processing Standards

1989. Prepared in cooperation with American National Standards Inst., New York,

Three ring vinyl binder also available; North American Continent price \$7.00; all others write for quote.

Keywords: \*Computer software, \*Federal information processing standard, Computer graphics, Fortran, Pascal programming language, Validation, Ada pro-gramming language, \*Graphic Kernel System, \*Language binding.

The report revision supersedes FIPS PUB 120 and modifies the standard by adding a requirement for validation of GKS implementations that are acquired by Federal agencies. FIPS 120-1 adopts American National Standard Graphical Kernel System (ANS GKS), ANSI X3.124-1985, Functional Description, which consists of four parts (X3.124.1-1985 FORTRAN Binding, X3.124.2-1988 Pascal Binding, X3.124.3-1989 Ada Binding), as a FIPS. ANS GKS specifies a library (or toolbox package) of subroutines for an application programmer to incorporate within a program in order to produce and manipulate two-dimensional pictures. The purpose of the standard is to promote portability of graphics application programs between different installations. The standard is for use by implementors as the reference authority in developing graphics software systems; and by other computer professionals who need to know the precise syntactic and semantic rules of the standard.

100,675 FIPS PUB 146-1 PC A05/MF A01 National Inst. of Standards and Technology (CSL),

Gaithersburg, MD.

Government Open Systems Interconnection Profile (GOSIP); Category: Hardware and Software Standards; Subcategory: Computer Network Protocols.

3 Apr 91, 81p Supersedes FIPS PUB 146.

Three ring vinyl binder also available: North American Continent price \$7.00; all others write for quote.

Keywords: \*Computer networks, \*Standards, Protocols, Specifications, \*Open systems interconnections, \*Federal information processing standards.

The publication is a revision of Federal Information Processing Standards (FIPS) 146 and supersedes FIPS 146 in its entirety. FIPS 146 adopted the Government Open Systems Interconnection Profile (GOSIP) which defines a common set of data communication protocols that enable systems developed by different vendors to interoperate and the users of different applications on those systems to exchange information. The revision contains all of the protocols in FIPS 146 plus additional protocols which provide new services useful to Federal agencies and increase the interoperability achievable among end systems of different manufacture. The revision also includes minor technical changes to the protocols in FIPS 146.

100,676 FIPS PUB 160 FIPS PUB 160 PC E15 National Inst. of Standards and Technology (NCSL), Gaithersburg, MD.

American National Standard for C. Category: Soft-

ware Standard. Subcategory: Programming Language. Final rept.

K. A. Miles. c1990, 361p

Also pub. as American National Standards Inst., New York rept. no. ANSI-X3.159-1989. Prepared in cooperation with American National Standards Inst., New York.

Three-ring vinyl binder also available: North American Continent price \$7.00; all others write for quote.

Keywords: \*Programming languages, Standards, Data processing, \*Federal Information Processing Standard, Information processing, Computer software, \*C programming language.

The publication announces the adoption of American National Standard for C, ANSI X3.159-1989, as a Federal Information Processing Standard (FIPS). The American National Standard for C specifies the form and establishes the interpretation of programs written in the C programming language. The purpose of the standard is to promote portability of C programs for use on a variety of data processing systems. The standard is for use by implementors as the reference authority in developing compilers, interpreters, or other forms of high level language processors; and by other computer professionals who need to know the precise syntactic and semantic rules adopted by ANSI.

100,677 FIPS PUB 161 PC A02 National Inst. of Standards and Technology (NCSL),

Gaithersburg, MD.
Electronic Data Interchange (EDI). Category: Software Standard. Subcategory: Electronic Data Interchange.

R. G. Saltman. 29 Mar 91, 10p

Three ring vinyl binder also available; North American Continent price \$7.00; all others write for quote.

Keywords: \*Data transmission, Electronics, Telecommunication, Businesses, \*Federal Information Processing Standard, \*Electronic data interchange.

The publication announces the adoption, as a Federal Information Processing Standard, of recognized na-tional and international standards for EDI. In EDI, data that would be traditionally conveyed on paper docu-ments are transmitted or communicated electronically according to established rules and formats. The data that are associated with each type of functional document, such as a purchase order or invoice, are transmitted together as an electronic message. The formatted data may be transmitted from originator to recipient via telecommunications or physically transported on electronic storage media.

100,678 FIPS PUB 54-1 PC F18 National Inst. of Standards and Technology (CSL),

Gaithersburg, MD.
Computer Output Microform (COM) Formats and Reduction Ratios, 16MM and 105MM. Category: Hardware Standard; Subcategory: Media.

Federal information processing standards (Final). T. C. Bagg. c15 Jan 91, 24p Supersedes FIPS PUB 54. Also pub. as American Na-

tional Standards Inst., New York rept. no. ANSI/AlIM-MS14-1988. Prepared in cooperation with American National Standards Inst., New York, and Association for Information and Image Management, Silver Spring,

Three ring vinyl binder also available: North American price \$7.00; all others write for quote.

Keywords: \*Microfilm, \*Standards, Data processing, Reduction, \*Federal information processing standards, \*Microform, \*Microfiche, Computer output micro-

The FIPS PUB specifies the image arrangement, size, and reduction ratios for 16mm and 105mm microforms generated by Computer Output Microfilmers. It is limited to systems using business-oriented fonts similar to line printer output. The revised FIPS adopts American National Standard for Information and Image Management -- Microfiche, ANSI/AIIM MS5-1991, and American National Standard for Information and Image Management -- Specifications for 16mm and 35mm Roll Microfilm, ANSI/AIIM MS14-1988.

PC A02/MF A01 FIPS PUB 9-1 National Inst. of Standards and Technology (NCSL), Gaithersburg, MD.

Congressional Districts of the United States. Category: Federal General Data Standard, Representations and Codes.

Federal information processing standards (Final).

H. Tom. 30 Nov 90, 10p Supersedes FIPS PUB 9.

Three ring vinyl binder also available, North American Continent price \$7.00; all others write for quote.

Keywords: \*United States, \*Congress, \*Federal Information Processing Standards, \*Specifications, Representation, Codes, Guidelines, \*Congressional Dis-

The standard provides the structure of numeric codes for representing congressional districts and similar areas defined for the various congresses of the United States. Congressional districts are legislatively defined subdivisions of a State for the purpose of electing representatives or delegates to the House of Representatives of the United States Congress. A State or equivalent entity may comprise a single congressional district or similar representational area.

FIPS SET 1991 PC\$2300.00 National Inst. of Standards and Technology, GaithersFederal Information Processing Standards Publication.

Federal Information Processing Standards.

1991, 2895p-in 162v Set includes FIPS PUB 0 through FIPS PUB 161 and 13 ring vinyl binders. Supersedes FIPS SET 1990.

Keywords: \*Computer Software, \*Federal Information Processing Standards.

No abstract available.

100.681 PB91-132126 PC A03/MF A01 National Inst. of Standards and Technology, Gaithersburg, MD.
Fed-X: The NIST Express Translator. Revised, No-

vember 1990.

S. N. Clark. Aug 90, 18p NISTIR-4371-REV See also PB90-269507.

Keywords: \*Translators, Parsers, Standards, \*Product data exchange, \*PDES(Product Data Exchange Specification), \*EXPRESS programming language, Software tools, Computer aided manufacturing.

The Product Data Exchange Specification (PDES) is an emerging standard for the exchange of product in-formation among various manufacturing applications. PDES includes an information model written in the Express language; other PDES-related information models are also written in Express. The National PDES Testbed at NIST has developed software to manipulate and translate Express models. This software consists of an in-memory working form and an associated Express language parser, FED-X. The design and capabilities of FED-X and the Express Working Form are discussed.

100.682 PB91-132159 PC A03/MF A01 National Inst. of Standards and Technology, Gaithersburg, MD. NIST PDES Toolkit: Technical Fundamentals. Na-

tional PDES Testbed Report Series (Revised). S. N. Clark. Nov 90, 34p NISTIR-4335/REV See also PB90-250093.

Keywords: Standards, Translators, \*Product data exchange, \*PDES(Product Data Exchange Specification), \*STEP(Standard for the Exchange of Product Model Data), \*Software tools, Computer aided manual Software tools, Computer aided manual Software tools, Computer aided manual Software tools, Computer and Publication facturing, Software libraries, Application programs(Computers), EXPRESS programming Ian-

The Product Data Exchange Specification (PDES) is an emerging standard for the exchange of product in-formation among various manufacturing applications. A software toolkit for manipulating PDES data has been developed at the National PDES Testbed at NIST. A technical overview of this PDES Toolkit is provided. Fundamental software libraries are described, and techniques for creating applications based on the Toolkit are discussed.

100 683 PC A03/MF A01 PB91-132183 National Inst. of Standards and Technology (NCSL), Gaithersburg, MD.
NIST Working Form for STEP: National PDES

Testbed Report Series (Revised). S. N. Clark. 19 Nov 90, 11p NISTIR-4351/REV

See also PB90-250044.

Keywords: \*Standards, \*Parsers, \*Product data exchange, \*PDES(Product Data Exchange Specification), \*STEP(Standard for the Exchange of Product Model Data), \*Computer aided manufacturing, Software tools

The Product Data Exchange Specification (PDES) is an emerging standard for the exchange of product information among various manufacturing applications. The neutral exchange medium for PDES product models is the STEP physical file format. The National PDES Testbed at NIST has developed software to manipulate and translate STEP models. This software consists of an in-memory working form and an associated physical file parser, STEPparse. The design and capabilities of STEPparse and of the STEP Working Form are discussed.

100,684 PB91-132209

PC A03/MF A01

# **Information Processing Standards**

National Inst. of Standards and Technology (NCSL),

Gaithersburg, MD.
Use of the IRDS Standard in CALS (Revised). D. K. Jefferson, and C. M. Furlani. Sep 89, 16p NISTIR-89-4169-REV See also PB90-112467.

Keywords: \*Information systems, \*Standards, \*Data base management systems, \*CALS(Computer aided Acquisition and Logistics Support), \*IRDS(Information Resource Dictionary System), Data dictionaries, Distributed data bases tributed data bases.

The objective of the point paper is to show how the Information Resource Dictionary System (IRDS) can fulfill critical design and operational requirements for CALS Phase II. First, a series of assumptions are made about the data management services which are needed by CALS Phase II. Next, these assumptions are used to develop a series of requirements for a dicitionary system. The structure of the IRDS family of standards is then described. Examples are provided to illustrate how the IRDS could meet the requirements. A schedule is presented to show that the IRDS and other data management standards will be available when needed to meet the immediate requirements of CALS. An architecture is presented to illustrate additional standards required to achieve longer-range goals of distributed database. Finally, development tasks are recommended.

100,685 PB91-134635 PB91-134635 Not available NTIS National Bureau of Standards (ICST), Gaithersburg, MD. Information Systems Engineering Div. Information Systems Engineering Program. Final rept.

Information systems Engineering Pro-Final rept.
F. E. Spielman. 1987, 3p
Pub. in Proceedings of International Conference on Interactive Information and Processing Systems for Meteorology, Oceanography, and Hydrology (3rd), New Orleans, LA., January 12-16, 1987, p58-60.

Keywords: \*Standards, \*Information systems, Programming languages, Computer graphics, Systems engineering, Reprints, \*Data bases, \*Data management, Data dictionaries, Data base management systems, Computer applications, National Institute of Standards and Technology.

Because of the increased use of packaged software for data management and applications development, there is a renewed interest in Federal, national, and international standards for database languages, data dictionary systems, computer graphics, data interchange, and interfaces to programming languages. Along with such specific standards, there is a need for guidance documents on data administration, logical database design, use of standard codes and represen-tations, selection of DBMS and graphics systems, and applications development. The presentation discusses applications overlopment. The presentation discusses the Information Systems Engineering program within the Institute for Computer Sciences and Technology (ICST) at the National Institute of Standards and Technology (NIST) and identifies standards, research activities, and guidance projects in these areas.

PC A99/MF A04 National Inst. of Standards and Technology (NCSL), Gaithersburg, MD.

Working Implementation Agreements for Open Systems Interconnection Protocols. T. Boland. Nov 90, 611p NISTIR-4448 See also PB90-259763. Presented at the NIST Workshop for Implementors of OSI Plenary Assembly, Gaithersburg, MD., September 14, 1990.

Keywords: \*Protocols, Standards, Computer networks, Message processing, File management systems, Computer security, Access, Data base management, Local area networks, \*OSI(Open Systems Interconnection), National Institute of Standards and Tech-

The document records Working Agreements on Implementation details of Open Systems Interconnection (OSI) Protocols among the organizations participating in the National Institute of Standards and Technology (NIST)/OSI Workshop Series for Implementors of OSI Protocols. These decisions are documented to facilitate organizaions in their understanding of the status of agreements. It is a standing document that is updated after each workshop (about 4 times a year).

100,687 PB91-158758

Not available NTIS

National Bureau of Standards (ICST), Gaithersburg, MD. Information Systems Engineering Div. Specifications for a Federal Information Processing Standard Data Dictionary System.

Final rept.
A. H. Goldfine. 1984, 13p
Pub. in Proceedings of NASA Administrative Data
Base Management Systems Conference, Greenbelt,
MD., May 25-26, 1983, p121-133 1984.

Keywords: \*Federal information processing standards, \*Data dictionaries, Data base management systems, Computer software, Specifications, Reprints.

The paper describes the data dictionary software specifications being developed by the Institute for Computer Sciences and Technology. The functionality and user interfaces in the final specifications will be incorporated into a planned Federal Information Processing Standard (FIPS) Data Dictionary System. The paper also discusses the focus and status of the effort to develop the planned FIPS DDS.

100,688 PB91-158915 PB91-158915 Not available NTIS National Bureau of Standards (ICST), Gaithersburg, MD. Systems and Network Architecture Div. Features and Facilities of Estelle.

Final rept. R. J. Linn. 1986, 26p

Pub. in Protocol Specification, Testing and Verification, p271-296 1986.

Keywords: \*Standards, Protocols, Pascal programming language, Specifications, Finite state machines, Reprints, \*Estelle, \*Data communications, ISO(International Organization for Standardization).

Estelle is a formal description technique developed by the International Organization for Standardization (ISO) in collaboration with the International Telegraph and Telephone Consultative Committee (CCITT). It is a draft proposed standard within ISO. Estelle was developed to be used by standards committees for the specification of data communications protocols which are destined to become international standards. A specification in Estelle is comprised of a set of modules which communicate with each other. Modules are specified as extended finite state machines using fa-cilities in Estelle which consist of a set of extensions to ISO Pascal.

100,689 PB91-171967 PC A99/MF E06 National Inst. of Standards and Technology (BFRL),

Gaithersburg, MD.
Stable Implementation Agreements for Open Systems Interconnection Protocols. Version 4, Edition

tems Interconnection Protocols. Version 4, Edition 1, December 1990.
Special pub. (Final).
T. Boland. Mar 91, 803p NIST/SP-500/183
Also available from Supt. of Docs. as SN903-015-00000-4. Supersedes PB90-212192.
Based on the Proceedings of the NIST Workshop for Implementors of OSI. Held in Gaithersburg, Maryland.

Keywords: \*Protocols, \*Computer communications, \*Computer networks, Standards, Agreements, Local area networks, Access methods, Message processing, Computer security, File management systems, Directories, Data base management systems, \*OSI(Open Systems Interconnection).

The document records current Stable Agreements for Open Systems Interconnection (OSI) Protocols among the organizations participating in the National Institute of Standards and Technology/OSI Workshop Series for Implementors of OSI Protocols.

100,690 PB91-187542 PC A03/MF A01
National Inst. of Standards and Technology (NCSL),
Gaithersburg, MD. Advanced Systems Div.
Standard Reference Materials Calling. Standard Reference Materials: Calibration of NIST Standard Reference Material 3201 for 0.5 Inch (12.65 mm) Serial Serpentine Magnetic Tape Car-

Special pub. (Final).
M. P. Williamson, N. E. Willman, and D. S. Grubb.
Feb 91, 39p NIST/SP-260-115
Also available from Supt. of Docs. as SN003-003-

Keywords: \*Magnetic tapes, \*Standards, Calibration, Test methods, \*Standard reference materials.

The publication describes the test system design and operation for the calibration of the NIST secondary

standard reference tapes SRM 3201 for 0.5 inch (12.65mm) 22 and 48 track serial serpentine magnetic tape cartridges. The importance of producing a Standard Reference Material for the magnetic tape cartridge is to promote the ability to interchange data both within and among various computer installations. Reliable interchange is assured when the media is designed and manufactured on the basis of a comparison to a known and accepted standard reference media.

100,691 PB91-197004 PC A11/MF A02 National Inst. of Standards and Technology, Gaithers-

Stable Implementation Agreements for Open Systems Interconnection Protocols. Version 4, Edition 1, March 1991. Change Pages (Supplement).

1, March 1991. Change rages (Supplication).
Special pub. (Final).
T. Boland. Jun 91, 236p NIST/SP-500/183SUPPL1
Also available from Supt. of Docs. as SN903-015-00000-4. See also PB91-171967.

Keywords: \*Protocols, Changes, Computer networks, Message processing, File management systems, Computer security, Data processing security, Algorithms, \*OSI(Open Systems Interconnection), National Institute of Standards and Technology.

The document records current Stable Agreements for Open Systems Interconnection (OSI) Protocols among the organizations participating in the National Institute of Standards and Technology (NIST)/OSI Workshop Series for Implementors of OSI Protocols.

100,692 PB91-201004 PC A05/MF A01 National Inst. of Standards and Technology (CSL), Gaithersburg, MD.

Application Portability Profile (APP): The U.S. Government's Open Systém Environment Profile OSE/ 1 Version 1.0.

Special pub. (Final). G. Fisher. Apr 91, 78p NIST/SP-500/187 Also available from Supt. of Docs.

Keywords: \*Computer applications, \*Computer program portability, \*Specifications, Computer program transferability, Protocols, Data structures, National government, United States, Information systems, Federal agencies, \*Open System Environment, \*APP(Application Portability Profile), National Institute of Standards and Technology. of Standards and Technology.

An Open System Environment (OSE) encompasses the functionality needed to provide interoperability, portability, and scalability of computerized applications across networks of heterogeneous hardware/software platforms. The OSE forms an extensible framework that allows interfaces, services, protocols, and supporting data formats to be defined in terms of nonproprietary specifications that evolve through open (public), consensus-based forums. A selected suite of specifications that define these interfaces, services, protocols, and data formats for a particular class or domain of applications is called a profile. The Application Portability Profile (APP) is the U.S. Government's OSE profile. It was developed to provide functionality across a broad range of Federal applications. The report describes the service areas and components included in the APP and provides evaluations of recommended specifications for the majority of the service area components. Organizations should use the report to assist in determining which specifications may be applicable to their particular environments.

PB91-203133 Not available NTIS National Inst. of Standards and Technology (NCSL), Gaithersburg, MD. Systems and Software Technology How the Government Shapes UNIX Standards.

Final rept. J. A. Hall. 1989, 1p Pub. in UNIX World 6, n4 p87(2) Apr 89.

Keywords: \*UNIX(Operating system), \*Federal information processing standards, Reprints, APP(Applications Portability Profile), POSIX(Portable Operating System Interface for Computer Environments), National Institute of Standards and Technolo-

The National Institute of Standards and Technology (NIST) is actively supporting standards developing activities relating to the Applications Portability Profile

### Information Processing Standards

(APP). A major component of the APP is POSIX (the Portable Operating System Interface for Computer Environments), and its relationship to the UNIX operating system.

100,694

PB92-110105 PC A05/MF A01 National Inst. of Standards and Technology (CSL), Gaithersburg, MD.

GOSIP Conformance and Interoperation Testing and Registration.

J. S. Nightingale. Mar 91, 94p NISTIR-4594 See also FIPS PUB 146-1 and PB91-187716.

Keywords: \*Federal information processing standards, \*Government procurement, \*Computer networks, Protocols, Acquisition, Computer communications, Computer program verification, Tests, Message processing, \*GOSIP(Government Open Systems Interconnection Profile).

The development of Federal Information Processing Standard (FIPS) 146 which specifies the Government Open Systems Interconnection Profile (GOSIP) resulted in the need to establish policy and procedures aimed at ensuring that Federally procured data communications products adhere to the technical documents referenced by GOSIP and that they interoperate. The goal of the report is to aid a Federal Acquisition. tion Authority in procurement of GOSIP products by employing publicly accessible registers verifying sup-plier claims of conformance and documenting in-stances of interoperability of GOSIP conformant prod-

100,695

PB92-112200 PC A04/MF A01 National Inst. of Standards and Technology (CSL), Gaithersburg, MD.

Stable Implementation Agreements for Open Systems Interconnection Protocols. Version 4, Edition 1, June 1991 Change Pages (Supplement). Final rept.

T. Boland, and B. Gray. Sep 91, 68p NIST/SP500-

Also available from Supt. of Docs. as SN903-015-00000-4. See also PB91-171967 and PB91-197004.

Keywords: \*Protocols, \*Computer communications, \*Computer networks, Standards, Changes, Agreements, Local area networks, Message processing, File management systems, Directories, \*OSI(Open Sys-tems Interconnection), NIST.

The document records current Stable Agreements for Open Systems Interconnection (OSI) Protocols among the organizations participating in the National Institute of Standards and Technology (NIST)/OSI Workshop Series for Implementors of OSI Protocols.

PB92-119676 PC A08/MF A02 National Inst. of Standards and Technology (CSL), Gaithersburg, MD.

Government Open Systems Interconnection Profile Users' Guide, Version 2.

Final rept. T. Boland. Oct 91, 167p NIST/SP-500/192 Also available from Supt. of Docs. Supersedes PB90-111212. See also PB91-171967, PB91-197004, PB92-112200 and FIPS PUB 146-1.

Keywords: \*Protocols, \*Computer communications, \*Computer networks, Standards, Message processing. OSI(Open Systems Interconnection), ing, OSI(Open Systems interconnection), \*GOSIP(Government Open System Interconnection), Federal agencies.

The document assists Federal agencies in planning for and procuring OSI. It provides tutorial information on OSI Protocols as well as information on OSI Registration, GOSIP Technical Evaluation, and GOSIP Transition Strategies.

100,697

PB92-126408 PC A11/MF A03 National Inst. of Standards and Technology (CSL), Gaithersburg, MD.

Stable Implementation Agreements for Open Systems Interconnection Protocols. Version 4, Edition 1, Change Pages September 1991. Output from the September 1991 OSI Implementors Workshop. Held in Gaithersburg, Maryland.

T. Boland. Nov 91, 242p NIST/SP500-183 3 Also available from Supt. of Docs. as SN903-015-00000-4. See also PB91-171967, PB91-197004 and PB92-112200.

Keywords: \*Protocols, Computer networks, Local area networks, \*OSI(Open System Interconnection), National Institute of Standards and Technology.

The document records current Stable Agreements for Open Systems Interconnection Protocols among the organizations participating in the NIST/OSI Implementors Workshop series.

100,698

PB92-126523 PC A17/MF A04 National Inst. of Standards and Technology (NCSL), Gaithersburg, MD.

Gailnersourg, MD. Working Implementation Agreements for Open Systems Interconnection Protocols.

T. Boland, Mar 91, 394p NISTIR-4507
Proceedings of the NIST workshop held in Gaithersburg, MD., December 14, 1990. See also PB91-1444444.

Keywords: \*Protocols, Standards, Computer networks, Message processing, File management systems, Local area networks, \*OSI(Open Systems Interconnection), National Institute of Standards and Tech-

The document records Working Implementation Specification Agreements of Open Systems Interconnection Protocols among the organizations participating in the NIST/OSI Workshop Series for Implementors of OSI Protocols. These decisions are documented to assist organizations in their understanding of the status of agreements. This is a standing document that is updated after each workshop (about 4 times a year).

PB92-126580 PC A05/MF A01 National Inst. of Standards and Technology (CSL),

Gaithersburg, MD.
Guidelines for the Evaluation of File Transfer,
Access and Management Implementations.

P. Markovitz, S. Trus, and C. Royster. Oct 91, 85p NIST/SP-500/196

Also available from Supt. of Docs. See also PB90-111212, PB91-171967, PB91-107565 and PB92-110105. Sponsored by Army Information Systems Command, Fort Huachuca, AZ., Air Force Communications Command, Scott AFB, IL., and Internal Revenue Service, Washington, DC.

Keywords: \*Computer network, \*Computer communications, File management systems, Access methods, \*OSI(Open Systems Interconnection).

The document advances the goals of the Government Open Systems Interconnection Profile (GOSIP) by providing guidelines for evaluating File Transfer, Access viding guidelines for evaluating File Transfer, Access and Management (FTAM) implementations. These guidelines can assist a user in determining which implementation, among several candidates, will best meet the functional and performance requirements of that user. Specifically, the document contains: (1) guidelines for evaluating the functional specifications of FTAM implementations, (2) guidelines for measuring the performance of FTAM implementations, and (3) guidelines for matching the functional and performance specifications of an FTAM implementation to the functional and performance requirements of the user. functional and performance requirements of the user.

### **Pattern Recognition & Image Processing**

100 700

PB91-216630 PC A03/MF A01 National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Robot Systems Div.

Real-Time Model-Based Tracking Combining Spatial and Temporal Features.

K. Chaconas, and M. Nashman. Jun 91, 24p NISTIR-

4610

Keywords: \*Tracking(Position), Moving targets, Real time, Correlation, Algorithms, \*Robot vision.

The paper describes a method for tracking moving image features by combining spatial and temporal edge information with model based feature information. The algorithm updates the two-dimensional posi-tion of object features by correlating predicted model features with current image data. The results of the correlation process are used to compute an updated model. The algorithm makes use of a high temporal sampling rate with respect to spatial changes of the image features and operates in a real-time multi-proc-essing environment. Preliminary results demonstrate successful tracking for image feature velocities be-tween 1.1 and 4.5 pixels every image frame.

100,701

PB92-112275 PC A03/MF A01 National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Robot Systems Div. Integration-Based Method for Depth Estimation. D. Raviv. Sep 91, 24p NISTIR-4669 Prepared in cooperation with Florida Atlantic Univ.,

Boca Raton.

Keywords: \*Image reconstruction, \*Depth finding, Computer vision, Three dimensional, Edge detection, Motion, Algorithms.

closed-form, integration-based, and massively-parallel algorithm for determining depth of points in 3-D using one moving camera is presented. It is based on analyzing a sequence of images that result from a known rectilinear motion of a camera (with no rotation) in a stationary environment. A traceable point in an image sequence is reconstructed using an integration operation (no differentiation operator is involved). The method arose from two simple observations: (1) Stationary points in the 3-D scene appear to move away from the focus of expansion (FOE); (2) The distance of a point in 3-D space from the camera motion-axis is the same at all instants of time. Any visible moving point in the image can be processed independently of, and concurrently with, any other point. Laboratory results for the case where the optical axis is parallel to the motion axis show an error of less than 0.6% in absolute distance.

100.702 PB92-112507 PC A03/MF A01 National Inst. of Standards and Technology, Gaithers-

burg, MD. Three Dimensional Reconstruction from Optical

Flow Using Temporal Integration. R. Rangachar, T. H. Hong, M. Herman, and R. Luck. Apr 91, 14p NISTIR-4570

Prepared in cooperation with American Univ., Washington, DC., Maryland Univ., College Park. Dept. of Mechanical Engineering, and Aspex, Inc., New York.

Keywords: \*Image reconstruction, Three dimensional, Image segmentation, Optical flow, Temporal integration, PIPE(Pipelined Image Processing Engine).

Image flow, the apparent motion of brightness patterns on the image plane, can provide important visual infor-mation such as distance, shape, surface orientation, and boundaries. It can be determined by either feature tracking or spatio-temporal analysis. The optical flow thus determined can be used to reconstruct the 3-D scene by determining the depth from camera of every point in the scene. However, the optical flow determined by either of the methods mentioned above will be noisy. As a result, the depth information obtained from optical flow can not be successfully used in practical applications such as image segmentation, 3-D re-construction, path planning, etc. By using temporal in-tegration, the accuracy of both the optical flow and the depth determined from optical flow can be increased. In the work, the authors describe an incremental integration scheme called the running average method to temporally integrate the image flow. They integrate the depth from camera obtained using optical flow determined from gradient based methods, and show that the results of temporal integration are much more useful in practical applications than the results from local edge operators. Finally, they consider an image segmentation example and show the advantages of temporal integration.

# Pattern Recognition & Image Processing

100,703 PB92-112564 PC A03/MF A01 National Inst. of Standards and Technology, Gaithers-

burg, MD.
Analysis of Optical Flow Estimation Using Epipolar Plane Images.
R. Rangachar, T. H. Hong, M. Herman, and R. Luck.
Apr 91, 14p NISTIR-4569
Prepared in cooperation with American Univ., Washington, DC., Maryland Univ., College Park. Dept. of Mechanical Engineering, and Aspex, Inc., New York.

Keywords: \*Image analysis, Image reconstruction, Edge detection, Distance, Motion, \*Optical flow, PIPE(Pipelined Image Processing Engine).

Image flow, the apparent motion of brightness patterns on the image plane, can provide important visual information such as distance, shape, surface orientation, and boundaries. It can be determined by either feature tracking or spatio-temporal analysis. The authors consider spatio-temporal methods, and show how differential range can be estimated from time-space imagery. The authors generate a time-space image by considering only one scan line of the image obtained from a camera moving in the horizontal direction at each time interval. At the next instant of time, the authors shift the previous line up by one pixel, and obtain an-other line from the image. The authors continue the procedure to obtain a time-space image, where each horizontal line represents the spatial relationship of the pixels, and each vertical line the temporal relationship. Each feature along the horizontal scan line generates an edge in the time-space image, the slope of which depends upon the distance of the feature from the depends upon the distance of the feature from the camera. The authors apply two mutually perpendicular edge operators to the time-space image, and determine the slope of each edge. The authors show that this corresponds to optical flow. The authors use the result to obtain the differential range, and show how this can be implemented on the Pipelined Image Processing Engine (PIPE). The authors use a simple technique to calibrate the comer and show how the details. nique to calibrate the camera and show how the depth can be obtained from optical flow. The authors provide a statistical analysis of the results of 3-D reconstruction of the scenes using optical flow determined from 3x3, 5x5, and 7x7 edge operators.

# General

100,704 PB91-148486 PC A09/MF A02 National Inst. of Standards and Technology (NCSL), Gaithersburg, MD.

Bibliography of Selected Computer Security Publi-

cations, January 1980-October 1989. Special pub (January 1980-October 1989). R. Turn, and L. E. Bassham. Dec 90, 200p NIST/SP-800/1

Contract 43NANB922203

Also available from Supt. of Docs. as SN003-003-03060-1. Prepared in cooperation with Turn (Rein) Associates, Pacific Palisades, CA.

Keywords: \*Computer security, \*Bibliographies, Access control, Data processing security, Computer privacy, Data bases, Computer networks, Cryptography, Secure communications, Auditing, Data integrity.

The bibliography cites selected books and articles on computer security published from January 1980 through October 1989. To have been selected, an article had to be substantial in content and have been published in professional or technical journals, magazines, or conference proceedings. Only very substantial articles from the popular or trade press were intal articles from the popular or trade press were included. English language articles from foreign journals were included as available. The citations are listed under nine categories. A tenth category of pre-1980 publications is also provided, as well as an appendix containing addresses of all journals and magazines referenced in the bibliography.

100 705 PB91-159228 Not available NTIS Mational Bureau of Standards (ICST), Gaithersburg, MD. Systems and Software Technology Div.

Thwarting the Hackers.

Final rept. E. F. Troy. 1984, 6p Pub. in Datamation, 6p, 1 Jul 84.

Keywords: \*Computer security, \*Access control, Comcommunications, Operating systems(Computers), Modems, Reprints.

The article provides general information about a new class of device designed to enhance communications security for computer systems. The 'port protection device' (PPD) is fitted on a computer's dial-up telephone line between the telephone set and the computer port, and operates independently of the computer. The PPD in its simplest form requires the dial-up user to supply a special password before gaining access to the computer line. Additional features described in the article include: camouflage of the port by initially hiding the characteristic modem tone; call-back to the authorized user telephone number for independent verification before connection; and logging of all activity on the line. The article includes a general table of characteristics for devices from the eleven known vendors, without performing any qualitative evaluation of them.

100.706 PB91-187740 PC A03/MF A01 National Inst. of Standards and Technology, Gaithersburg, MD. Computer Security: Selected Articles.

Internal rept.

M. Swanson, and E. Lennon. cApr 91, 46p NISTIR-

Keywords: \*Computer security, Local area networks, Risk, Computer viruses, Computer privacy, Data integ-rity, Data processing security, Computer software, Per-sonal computers, Data encryption, Computer networks, Internet.

Contents: Is Your System Safe; Proper assignment of responsibility for data security; Assessing Security; NIST Group Explores Risk-Assessment Packages; Crackdown on software pirates; Memo: Computer Viruses and Personal Computers; Reflections on Trusting Trust; The Science of Computing: The Internet Worm; and Secret Codes.

100,707 PB91-187781 PC A06/MF A01 National Inst. of Standards and Technology, Gaithersburg, MD.

National Aeronautics and Space Administration's (NASA) Automated Information Security Hand-

E. Roback. Mar 91, 107p NISTIR-4518, NHB-2410.9 Sponsored by National Aeronautics and Space Administration, Washington, DC. Information Resources Management Office.

Keywords: \*Data processing security, \*Handbooks, Risk assessment, Telecommunication, Microcomputers, NASA, \*Computer security, \*Information security, Automated Information Security programs, Accreditation Coefficiency ( tion, Contingency plans.

The National Aeronautics and Space Administration's (NASA) Automated Information Security Handbook provides NASA's overall approach to automated information systems security including discussions of such aspects as: program goals and objectives, assignment of responsibilities, risk assessment, foreign national access, contingency planning and disaster recovery, awareness training, procurement, certification, planning, and special considerations for microcomputers.

100,708 PB91-187864 PC A08/MF A01 National Inst. of Standards and Technology (CSL), Rational flist. Of Standards and Technology (Caithersburg, MD.

Public-Key Cryptography. Computer Security.
Special pub. (Final).

J. Nechvatal. Apr 91, 172p NIST/SP-800/2

Also available from Supt. of Docs. as SN003-003-

Keywords: \*Cryptography, \*Computer security, Cryptology, Data encryption, Data processing security, Computer information security, Data integrity, Access control, Secure communications, Authentication, Protocols, Local area networks, Algorithms, Computer ar-chitecture, \*Public-key systems, Digital signatures, Hash functions.

The paper surveys public-key cryptography. It discusses the theory of public-key cryptography and examines several examples of public-key cryptosystems. It also treats the related topics of digital signatures, hash functions, and, more briefly, zero-knowledge protocols. Modes of implementation of public-key crypto-

systems are discussed, including implementation in networks. Examples of existing or proposed implementations are summarized. Comparisons to secret-key cryptography are made. Relevant mathematics is covered in appendices. An extensive bibliography is in-

100,709

PB91-189571 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Semiconductor Electronics Div. Knowledge Verification of Machine-Learning Procedures Based on Test Structure Measurements. Final rept.

D. Khera, L. W. Linholm, R. A. Allen, M. W. Cresswell, V. C. Tyree, W. Hansford, and C. Pina.

Pub. in Proceedings of International Conference on Microelectronic Test Structures, Kyoto, Japan, March 18-20, 1991, p145-149.

Keywords: \*Machine learning, \*Knowledge bases(Artificial intelligence), Export systems, Systems engineering, Tests, Heuristic methods, Comparison, Reprints.

The paper describes an approach for evaluating and refining the rules, based on test structure measurements, to be entered into the knowledge base of an expert system that characterizes device performance. The objective is to qualify the performance of rules determined by a machine-learning classification applica-tion with the best knowledge available from the human experts. The technique combines a machine-learning approach with the traditional heuristic based development of an expert system. Strengths and weaknesses of the individual techniques are compared.

100.710

PB91-203380 Not available NTIS Mational Bureau of Standards (ICST), Gaithersburg, MD. Systems and Software Technology Div. Static Analysis Tools for Software Security Certifi-

cation. Final rept.

D. R. Kuhn. 1988, 9p

Pub. in Proceedings of the National Computer Security Conference (11th), October 17-20, 1988, p290-298.

Keywords: \*Computer software, \*Computer security, \*Software tools, Cryptography, Electronic funds transfer, Data encryption, Data processing security, Computer program verification, Reprints, Static analysis.

The paper describes a suite of tools used in evaluating software for security certification. The tools are currently being used on cryptographic software for secure Electronic Funds Transfer, but could be applied to other applications as well.

100 711

PB91-204107 Not available NTIS National Inst. of Standards and Technology (NCSL), Gaithersburg, MD. Computer Security Div. Data Encryption Standard: Past and Future. Final rept.

M. E. Smid, and D. K. Branstad. 1988, 10p Pub. in Proceedings of the IEEE (Institute of Electrical and Electronics Engineers) 76, n5 p550-559 1988.

Keywords: \*Data encryption, \*Standards, Cryptography, Algorithms, Data processing security, Electronic funds transfer, Reprints.

The Data Encryption Standard (DES) is the first, and to the present date, only, publicly available cryptographic algorithm that has been endorsed by the U.S. Government. The paper deals with the past and future of the DES. It discusses the forces leading to the development of the standard during the early 1970's, the controversy regarding the proposed standard during the mid 1970's, the growing acceptance and use of the standard in the 1980's, and some recent developments that could affect the future of the standard.

100.712

PB91-216671 PC A07/MF A02 National Inst. of Standards and Technology (CSL), Gaithersburg, MD.

#### General

Standard Security Label for GOSIP: An Invitational Workshop. Held on April 9-10, 1991. N. Nazario. Jun 91, 133p NISTIR-4614

Keywords: \*Meetings, \*Computer security, \*Standards, Protocols, United States government, Computer networks, Federal information processing standards, Data processing security, Government policies, Cryptography, Data integrity, \*GOSIP(Government Open Systems Interconnection Profile), National Institute of Standards and Technology, Security labels.

On April 9 and 10, 1991 the Protocol Security Group at On April 9 and 10, 1991 the Protocol Security Group at the National Institute of Standards and Technology (NIST) held its Second Workshop on Security Labels. Forty representatives from the U.S. Government, In-dustry, and the Canadian Government gathered for two days to discuss a NIST proposed Standard Security Label for the U.S. Government Open Systems Inter-connection Profile (GOSIP). Issues on security policy and security object registration were also discussed in reference to the proposed label. The information shared during the two days of discussion and the recommendations of the group are documented in the proceedings.

100,713

PB91-222638 PC A08/MF A02 National Inst. of Standards and Technology, Gaithers-

**Automated Information Systems Security Program** Handbook.

E. Roback. Jul 91, 156p NISTIR-4636 Reprinted with Permission by U.S. Department of

**Human Services** 

Keywords: \*Computer information security, \*Handbooks, Data processing security, Risk assessment, Personal computers, Word processing, Telecommuni-cation, \*Computer security, Contingency plans, US

The Interagency Report presents the U.S. Department of Health and Human Services' (HHS) Automated Information Systems Security Program Handbook which provides a comprehensive description of the program elements which comprise HHS's approach to computer security. Among the varied items included are: security policy and responsibilities, security level designators, security level requirements, security administration, risk management, contingency planning, person-nel security, facility security, application systems and data security, personal computers, data communications, and acquisitions and contracts.

100.714

PB91-237677 Not available NTIS
National Inst. of Standards and Technology (MEL),
Gaithersburg MD Pabet Systems Disc Gaithersburg, MD. Robot Systems Div.
Geometric Reasoning for Constructing 3D Scene

Descriptions for Images. Final rept.

L. Walker, and M. Herman. 1988, 16p Pub. in Artificial Intelligence 37, n1-3 p275-290 Dec 88.

Keywords: \*Computer vision, \*Three dimensional models, \*Image processing, Reasoning, Expert systems, Knowledge bases(Artificial intelligence), Robotics, Knowledge representation, Reprints.

There are many applications for a vision system which derives a three-dimensional model of a scene from one or more images and stores the model for easy retrieval and matching. The derivation of a 3D model of a scene involves transformations between four levels of representation: images, 2D features, 3D structures, and 3D geometric models. Geometric reasoning is and 3D geometric models. Geometric reasoning is used to perform these transformations, as well as for the eventual model matching. Since the image formation process is many-to-one, the problem of deriving 3D features from 2D features is ill-constrained. Additional constraints may be derived from knowledge of the domain from which the images were taken. The 3D Mosaic system has successfully used domain specific provided to drive the reometric reasoning necessary. knowledge to drive the geometric reasoning necessary to acquire 3D models for complex real-world urban scenes. To generalize this approach, a framework for the representation and use of domain knowledge for geometric reasoning for vision is proposed.

100,715

PB92-108893 PC A08/MF A02 National Inst. of Standards and Technology (CSL), Gaithersburg, MD.

Guide to Expert System Building Tools for Microcomputers. Special pub. (Final).

E. Dabrowski, and E. N. Fong. Jul 91, 151p NIST/

SP-500/188

Also available from Supt. of Docs. as SN003-003-

Keywords: \*Expert systems, \*Microcomputers, \*Systems engineering, \*Software tools, Knowledge bases(Artificial intelligence), Knowledge representation, Man computer interface, Computer software, Object-oriented programming.

Microcomputer-based expert system building tools (microcomputer-based ESBTs), sometimes known as expert system shells, are software packages for development of expert systems that run on microcomputers. The report provides system managers, planners, and potential expert system developers with a readable de-scription of ESBTs for microcomputers including a de-tailed description of specific tool features and the capabilities they support. The technical content of the report is based on analysis of commercially available ESBTs. However, individual commercial products are not described, compared, or ranked.

100,716 PB92-112259 PC A09/MF A02 National Inst. of Standards and Technology, Gaithersburg, MD.

Glossary of Computer Security Terminology. E. Roback. Sep 91, 177p NISTIR-4659

Keywords: \*Computer information security, \*Data processing security, \*Dictionairies, Computer security, Computer privacy.

The Glossary of Computer Security Terminology provides a summary of frequently encountered computer and communications security terms and various definitions used by federal agencies for those terms. The glossary does not provide a single definition per term; rather it reflects the variations in use of these terms among federal organizations.

PB92-112390 PC A03/MF A01 National Inst. of Standards and Technology (CSL), Gaithersburg, MD. Computer Security Div. Computer Security Bulletin Board System. User's

M. Skandera, and M. Swanson, Sep 91, 40p NISTIR-

Keywords: \*Computer information security, User manuals, Bulletin Board System, BBS system, Computer security, Computer privacy, US NIST.

The Computer Security Act of 1987 assigned to the National Institute of Standards and Technology (NIST) the responsibility for providing federal agencies with advice and assistance in the area of computer securi-ty. To accomplish a portion of the task, the NIST Com-puter Security Division maintains an electronic bulletin board system (BBS) which focuses on computer secu-rity issues. The NIST Computer Security BBS makes a wide variety of computer security information available to federal agencies and the public and encourages the sharing of information which can help users and managers protect their data and systems. The document describes the BBS and provides detailed instructions on how to use the many functions.

PB92-116391 PC A05/MF A01 National Inst. of Standards and Technology (CSL), Gaithersburg, MD. Security in ISDN.

Special pub. (Final). W. E. Burr. Sep 91, 77p NIST/SP-500/189 Also available from Supt. of Docs. as SN003-003-03112-7. See also PB90-198946 and N89-25634.

Keywords: \*Computer security, \*Computer networks, \*Communication networks, Standards, Access conrtol, Data encryption, Data processing security, Computer privacy, Data integrity, Protocols, \*ISDN(Integrated Services Digital Network), OSI(Open Systems Interconnection).

The Integrated Services Digital Network (ISDN) standards will provide worldwide digital communications service and will play a key role in the transition to electronic documents and business transactions. ISDN has been developed with little thought to security. ISDN security will become a pressing concern for both government and business. ISDN's digital nature facilitates adding security, but the deployment of ISDN in the public network is well under way and the present investment in ISDN equipment, as well as the commercial property to the public management. cial necessity to deploy ISDN in a timely manner, con-strains how security features may be added. ISDN se-curity standards should take advantage of, and be compatible with, emerging standards for Open Systems Interconnection (OSI) security. International Standard 7498-2 defines five security services for OSI: Confidentiality, Access Control, Authentication, Data Integrity and Non-repudiation. The challenge of ISDN security is to extend these concepts to all ISDN applications, including voice use of the public network. Ter-minal-to-terminal link encryption provides a powerful ISDN security mechanism, because of ISDN's ability to provide circuit switched connections throughout the world. A standard for the reliable authentication of human users is badly needed for ISDN security.

PB92-117068 Not available NTIS National Inst. of Standards and Technology (NCSL), Gaithersburg, MD.
Book Review: 'The Art of Computer Systems Per-

formance Analysis' by R. Jain.

Final rept.

G. Lyon. 1991, 2p Sponsored by Defense Advanced Research Projects

Agency, Arlington, VA.
Pub. in IEEE (Institute for Electrical and Electronics
Engineers) Design and Test of Computers, p90-91 Sep

Keywords: \*Computer systems performance, \*Computer performance evaluation, Reviews, Experimental design, Probability theory, Computerized simulation, Mathematical models, Statistical analysis, Queueing theory, Reprints.

The book covers a wide spectrum of performance topics. Its review is organized as follows: Overview. topics. Its review is organized as follows: Overview. Professional sources, projects, mistakes, techniques, metrics; Measurement. Workloads (type, selection, characterization), monitors, accounting logs, capacity planning, benchmarking, data presentation, honesty in comparisons; Probability and Statistics. Summarizing measured data, comparing systems, regressions (linear and other); Design of Experiments. Screening: 2 to the k power, 2 to the k power r factorials, 2 to the (k-p) power fractional factorials; Comparing: One-factor experiments, two-factor full factorials (without and with replication, r), full factorials (without and without and wit replication, r), full factorials with k factors; Simulation. Background, mistakes, verification, random numbers and their tests, random-variates, 20 common distributions; Queueing Models. Single queues, networks, operational laws, mean-value analysis, convolution, hierarchical decomposition.

PB92-123140 PC A03/MF A01 National Inst. of Standards and Technology (CSL),

National Inst. of Standards and Technology (CSL), Gaithersburg, MD.

Establishing a Computer Security Incident Response Capability (CSIRC).

Special pub. (Final).

J. P. Wack. Nov 91, 47p NIST/SP-800/3

Also available from Supt. of Docs as SN003-003-03121-6. See also PB90-115601.

Keywords: \*Computer information security, Data processing security, Computer viruses, Risk analysis, Threat evaluation, Vulnerability, \*CSIRC, Computer Security Incident Response Capabilities.

Government agencies and other organizations have begun to augment their computer security efforts be-cause of increased threats to computer security. Incidents involving these threats, including computer viruses, malicious user activity, and vulnerabilities asso-ciated with high technology, require a skilled and rapid response before they can cause significant damage. These increased computer security efforts, described here as Computer Security Incident Response Capa-bilities (CSIRCs), have as a primary focus the goal of reacting quickly and efficiently to computer security incidents. CSIRC efforts provide agencies with a centralized and cost-effective approach to handling computer security incidents so that future problems can be effi-ciently resolved and prevented. While the risks to computer security have increased, agencies have also become more dependent on computers. Many systems in widespread use today do not contain safe-guards to guarantee protection from these threats. Ad-

ditionally, as systems become more complex, they are more prone to vulnerabilities that can increase the risk of malicious exploitation. Due to greater availability of computers, users are often de facto system managers, however many have neither the requisite skills nor time however many have neither the requisite skills nor time to manage their systems effectively. These factors make it clear that agencies need to augment their computer security capabilities before they suffer from serious computer security problems that can harm their missions, result in significant expense, and tarnish their images. A CSIRC can help agencies resolve computer security problems in a way that is both efficient and cost-effective. Combined with policies for centralized reporting, a CSIRC can reduce waste and duplication while providing a better posture against poduplication while providing a better posture against po-tentially devastating threats. A CSIRC is a proactive approach to computer security, one that combines reactive capabilities with active steps to prevent future incidents from occurring.

# **DETECTION &** COUNTERMEASURES

### **Magnetic Detection**

100,721 AD-A230 438/4 PC A02/MF A01 National Inst. of Standards and Technology (NEL), Boulder, CO. Electromagnetic Fields Div. Summary of Experiments with the Separated Aperture Technique of Dielectric Anomaly Detection. Final rept. F. R. Clague. Dec 89, 8p Rept no. SR-723-29-89

Keywords: Anomalies, Antennas, \*Antipersonnel mines, \*Countermeasures, Cross polarization, \*Detection, Dielectrics, Holography, Horn antennas, Images, Intrusion, Measurement, \*Mine detectors, Narrowband, Plates, Time domain.

This report summarizes experiments conducted for the Mine Detection Division, Counter-Mine, Counter-Intrusion Department. The objective of this report is to provide a condensed overview of the major things tried, with an indication of how well they worked, and a reference to the original report that will allow finding the more detailed description if desired. The objective of the experiments was to study and improve what has generally been called the separated aperture system of dielectric anomaly detection. The detection portion of the system is a 'head' made of a transmit antenna and a receive antenna separated by a flat plate called the 'septum'. While the items tested were primarily the different versions of the separated aperture heads, a small number of other antennas was also evaluated. These included broadband horns used for time domain measurements, a narrow band horn used for holographic imaging, and cross polarized antennas that were used in an antipersonnel mine detector.

### **Radiofrequency Detection**

PB91-143347 PC A03/MF A01 National Inst. of Standards and Technology (NEL), Boulder, CO. Electromagnetic Fields Div. Near-Field and Far-Field Excitation of a Long Con-

ductor in a Lossy Medium.

D. A. Hill. Sep 90, 38p NISTIR-3954
Sponsored by Army Belvoir Research Development and Engineering Center, Fort Belvoir, VA.

Keywords: \*Magnetic fields, \*Electric conductors, Electric fields, Field strength, Far fields, Near fields, Electric dipoles, Line current, Plane waves, Excitation, Funnels, Grounded conductors, Insulated conductors, Underground conductors, Electromagnetic detection.

Excitation of currents on an infinitely long conductor is analyzed for horizontal electric dipole or and for a plane-wave, far-field source. Any of these

sources can excite strong currents which produce strong scattered fields for detection. Numerical results for these sources indicate that long conductors produce a strong anomaly over a broad frequency range. The conductor can be either insulated or bare to model ungrounded or grounded conductors.

# **ELECTROTECHNOLOGY**

#### **Antennas**

100.723

PB91-132274 PC A07/MF A01 National Inst. of Standards and Technology (NEL), Boulder, CO. Electromagnetic Fields Div. Spherical Near-Field Scanning: Experimental and

Theoretical Studies.
R. C. Wittmann, and C. F. Stubenrauch. Jul 90, 127p

NISTIR-3955

Sponsored by Rome Air Development Center, Hanscom AFB, MA. Electromagnetics Directorate.

Keywords: Spherical harmonics, Spherical waves, Far field, Algorithms, \*Antenna measurements, Microstrip antennas, Probes(Electromagnetic), Near field.

The report documents the evaluation of spherical near-field scanning algorithms and computer code developed at the National Institute of Standards and Technology. The experimental work is primarily a comparison of probe-compensated spherical and planar near-field measurement results for a common test antenna. Theoretical work is largely supportive of the experimental effort, but some peripheral topics are developed: For example, (1) application of spherical nearfield measurements to the determination of incident fields in compact ranges; and, (2) spherical-wave expansions for the fields of a uniformly excited circular aperture (to facilitate the creation of analytic test data).

100,724

PB91-134239 Not available NTIS National Inst. of Standards and Technology (NEL), Boulder, CO. Electromagnetic Fields Div.

Calibration of Antenna Factor at a Ground Screen Field Site Using an Automatic Network Analyzer. Final rept.

E. B. Larsen, R. L. Ehret, D. G. Camell, and G. H. Koepke. 1989, 6p

Sponsored by Naval Air Systems Command, Washing-

Pub. in Proceedings of IEEE (Institute of Electrical and Electronics Engineers) National Symposium on Electromagnetic Compatibility, Denver, CO., May 23-25, 1989, p19-24,

Keywords: \*Antennas, \*Electromagnetic fields, \*Network analyzers, \*Test facilities, Electromagnetic radiation, Field strength, Antenna radiation patterns, Amplification, Dipoles, Reprints, \*Calibration.

The technique now employed at the National Institute of Standards and Technology (NIST) for calibrating antenna factor at frequencies from 25 to 1000 MHz uses a standard open-circuit half-wave receiving dipole to measure the electric field strength. Unfortunately, the dipole responds to ambient fields over a large frequency range. This approach is compared with a three-an-tenna method which uses an accurate automatic network analyzer with 120 dB dynamic range to measure insertion loss between the transmitting and receiving antennas. A field site having a 20 m  $\times$  60 m ground screen which acts as a good reflector is used.

100.725

PB91-148239 Not available NTIS National Inst. of Standards and Technology (NEL), Boulder, CO. Electromagnetic Fields Div. Spherical Near-Field Scanning: Determining the Incident Field Near a Rotatable Probe.

Final rept.

R. C. Wittman. 1990, 4p Pub. in Proceedings of Antennas and Propagation Symposium Digest, Dallas, TX., May 7-11, 1990, p224-

Keywords: Probes(Electromagnetic), Electromagnetic compatibility, Electromagnetic interference, Near field, Scanning, Algorithms, Reprints, \*Antenna measurements

Many RCS, EMI/EMC, and antenna measurements require a known incident field within a test volume. To evaluate systems designed to produce a specific inci-dent field (compact ranges, for example), one must measure the actual illumination for comparison with design specifications. Beyond its diagnostic value, this incident field data can also be used for error estimation and for calculating first order corrections. In the paper, the author develops a spherical near-field scanning algorithm for determining incident fields inside a probe's 'minimum sphere.' This differs from the well-known spherical near-field scanning formulation which determines fields outside the source's minimum sphere. The scanner size depends on the extent of the region of interest and not on the extent of the (possibly much larger) source. The data may be collected using a standard roll-over-azimuth positioner.

100,726

PB91-185124 PC A03/MF A01 National Inst. of Standards and Technology (NEL), Boulder, CO. Electromagnetic Fields Div. NIST Calibration Procedure for Vertically Polarized

Monopole Antennas 30 kHz to 300 MHz. Technical note.

D. G. Camell, E. B. Larsen, J. E. Cruz, and D. A. Hill.

Jan 91, 26p NIST/TN-1347 Also available from Supt. of Docs. as SN003-003-03077-5.

Keywords: \*Monopole antennas, \*Calibration, Low frequency, Medium frequency, High frequency, Very high frequency, Polarization, Antenna factors.

The report describes the theoretical basis and test procedure for vertically polarized monopole antenna calibrations at the National Institute of Standards and Technology (NIST). The standard field method applies the theoretical equations of a vertical monopole antenna to calculate the vertical electric field. The method is used at the NIST open field site in the frequency range of 30 kHz to 300 MHz. The uncertainty in the antenna factor of the antenna under test (AUT) is now + or - 1

100.727

PB91-236919 Not available NTIS National Inst. of Standards and Technology (NEL), Boulder, CO. Electromagnetic Fields Div.

Alignment Fixture for Millimeter Waveguide.

Final rept.

D. P. Kremer, and A. C. Newell. 1990, 4p Pub. in IEEE (Institute of Electrical and Electronics Engineers) Antennas and Propagation Society Magazine 32, n3 p45-48 Jun 90.

Keywords: \*Antennas, Millimeter waves, Alignment, Fixtures, Reprints, \*Waveguide flanges.

Millimeter wave measurements require that care be exercised in the connection and handling of the waveguide flanges and their contact surfaces. When properly connected these flanges can provide many years of reliable and repeatable measurements. Improper use will limit the flange use to just a few connections, and result in large measurement errors. These errors are especially acute in situations requiring repeated connecting and disconnecting of these flanges, such as in antenna or insertion loss measurements. Several factors contribute to these errors, but the largest are improperly installed waveguide flanges, misalignment in flange connections, and excess strain on the waveguide or the flange. The National Institute of Standards and Technology has addressed these problems by developing a mechanical alignment fixture for millimeter band waveguide. Two fixtures were developed; one for small devices such as standard gain horns which can be supported by the fixture and another for larger devices. These systems along with a properly installed flange can reduce the uncertainty of the connection from greater than 1 dB to a few hundredths of a deci-

100,728

PB91-237073 Not available NTIS National Inst. of Standards and Technology (EEEL), Boulder, CO. Electromagnetic Fields Div.

### Antennas

General Technique to Correct Probe Position Errors in Planar Near-Field Measurements to Arbitrary Accuracy.

Final rept.

L. A. Muth, and R. L. Lewis. 1990, 8p

Pub. in IEEE (Institute of Electrical and Electronics Engineers) Transactions on Antennas and Propagation 38, n12 p1925-1932 Dec 90.

Keywords: \*Antennas, Probes(Electromagnetic), Taylors series, Error analysis, Near field, Far field, Re-

A general theoretical procedure is presented to remove known probe position errors when planar near-field data are transformed to the far field. The authors represented the measured data as a Taylor series, whose terms contain the error function and the ideal spectrum of the antenna. This representation is then assumed to be an actual near field existing on an error free regularly spaced two dimensional scan plane. Then by inverting the Taylor series, they obtain the ideal spectrum in terms of the measured data and the position errors. The solution is given by an infinite series of an error operator acting on data containing errors of measurement. The error operator is the Taylor series without the zeroth-order term. The nth order approximation to the ideal near field of the antenna can be explicitly constructed by inspection of the structure of the error operator.

PB92-110279

(Order as PB92-110261, PC A05/MF A01) National Inst. of Standards and Technology, Boulder, CO.

General Analytic Correction for Probe-Position Errors in Spherical Near-Field Measurements.

L. A. Muth. c1991, 20p Included in Jnl. of Research of the National Institute of Standards and Technology, v96 n4 p391-410 Jul/Aug

\*Antenna Keywords: radiation patterns, Probes(Electromagnetic), Computerized simulation, Spherical configuration, Near field, Correction, Graphs(Charts).

A general theoretical procedure is presented to remove known probe-position errors in spherical near-field data to obtain highly accurate far fields. The measured data is represented as a Taylor series in terms of the displacement errors and the ideal spectrum of the antenna. The representation is then assumed to be an actual near field on a regularly spaced error-free spherical grid. The ideal spectrum is given by an infinite series of an error operator acting on data containing errors of measurement. This error operator is the Taylor series without the zeroth-order term. The nth-order approximation to the ideal near field of the antenna can be explicitly constructed by inspection of the error operator. Computer simulations using period-ic error functions show that the authors are dealing with a convergent series, and the error-correction technique is highly successful.

100 730

PB92-112283 PC A04/MF A01 National Inst. of Standards and Technology (EEEL), Boulder, CO. Electromagnetic Fields Div. Personal Computer Codes for Analysis of Planar Near Fields.

L. A. Muth, and R. L. Lewis. Jun 91, 64p NISTIR-3970

Sponsored by Air Force Guidance and Metrology Center, Newark AFS, OH.

Keywords: \*Antenna radiation patterns, Data management, Personnel computers, Computer applications, Near field, Far field, Metrology, Computation, Subroutines, Fortran, PNFC codes.

Fortran codes were developed for analysis of planar near-field data. The report describes some of the inner workings of the codes, the data management schemes, and the structure of the input/output sections to enable scientists and programmers to use these codes effectively as a research tool in antenna metrology. The open structure of the codes allows a user to incorporate into the package new applications for future use with relative ease. The subroutines currently in existence are briefly described, and a table showing the interdependence among these subrou-tines is constructed. Some basic research problems, such as transformation of a near field to the far field and correction of probe position errors, are carried out

from start to finish to illustrate use and effectiveness of these codes. Sample outputs are shown. The advantage of a high degree of modularization is demonstrated by the use of DOS batch files to execute FORTRAN modules in a desired sequence.

#### Circuits

100.731

PB91-148700 Not available NTIS National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div.
High Speed Superconducting A/D Converter.

Final rept.

C. A. Hamilton, F. L. Lloyd, and R. L. Kautz. 1984, 4p Contract N00014-83-F-0012 Sponsored by Office of Naval Research, Arlington, VA.

Pub. in Proceedings of Government Microcircuit Applications Conference, Las Vegas, NV., November 6-8, 1984, p140-143.

Keywords: \*Analog to digital converters, \*Superconducting devices, Signal processing, Reprints.

Superconducting electronics has demonstrated impressive performance capabilities for small digital systems and analog signal processing applications. One of the areas where superconductivity offers a unique advantage is in ultra-high speed A/D conversion. The paper describes the operation and current status of a 6-bit, 4 gigasample/second A/D converter which has been developed at NBS.

100,732

PB91-149310 Not available NTIS Mational Inst. of Standards and Technology (NEL), Gaithersburg, MD. Electricity Div. Comprehensive Approach for Modeling and Testing Analog and Mixed-Signal Devices. Final rept. T. M. Souders, and G. N. Stenbakken. 1990, 8p

Pub. in Proceedings of International Test Conference, Washington, DC., September 10-14, 1990, p169-176

Keywords: \*Models, \*Tests, Analog to digital converters, Optimization, Computer software, Reprints, ers, Optimization, Computer softwa \*Analog devices, \*Mixed-signal devices.

An approach is presented for optimizing the testing of analog and mixed-signal devices. The entire process is performed with algebraic operations on an appropriate model. The paper demonstrates how this is accomplished using simple calls with public-domain software. Examples of test results achieved using this approach are included.

100,733

PB91-149401 Not available NTIS National Inst. of Standards and Technology (NEL),

Gaithersburg, MD. Electricity Div.
Device for Audio-Frequency Power Measurement. Final rept.

G. Q. Tong, Z. T. Qian, X. Y. Xu, and L. X. Liu. 1990,

Pub. in IEEE (Institute of Electrical and Electronics Engineers) Transactions on Instrumentation and Measurement 39, n3 p540-544 Jun 90.

Keywords: \*Power measurement, Electric current meters, Voltage measuring instruments, Audio fre-\*Power measurement. Electric current quencies, Reprints.

A new device for the measurement of audio-frequency power is introduced. The device can also be used to measure audio-frequency voltage and current. The full range of power factors are accomodated (cos theta = 0 to 1). Voltage and current measuring ranges are 15-600 V and 0.1-10 A, respectively. When cos theta = 1, the permissible error of the power measurement is from 50 to 150 ppm over the frequency range of 40 Hz to 10 kHz (including the line power frequency).

100,734

PB91-236554 Not available NTIS National Inst. of Standards and Technology (EEEL), Gaithersburg, MD. Electricity Div. Investigating the Use of Multimeters to Measure Quantized Hall Resistance Standards. Final rept.

M. E. Cage, D. Y. Yu, B. M. Jeckelmann, R. L. Steiner, and R. V. Duncan. 1991, 5p See also PB91-101097.

Pub. in IEEE (Institute of Electrical and Electronics Engineers) Transactions on Instrumentation and Measurement 40, n2 p262-266 Apr 91.

Keywords: \*Electrical resistance, \*Multimeters, \*Standards, Josephson junctions, Calibration, Resis-tors, Accuracy, Reprints, \*Quantum Hall effect, \*Re-sistance standards, Josephson arrays.

A new generation of digital multimeters was used to compare directly the ratios of the resistances of several wire-wound resistors and a quantized Hall resistor. The accuracies are better than 0.1 ppm for ratios as large as 4:1 if the multimeters are calibrated with a Josephson array.

100,735

PB91-236802 Not available NTIS National Inst. of Standards and Technology (EEEL), Gaithersburg, MD. Electricity Div. RF-DC Differences of Thermal Voltage Converters

Arising from Input Connectors.

Final rept. D. X. Huang, J. R. Kinard, and G. Rebuldela. 1991,

See also PB91-101295.

Pub. in IEEE (Institute of Electrical and Electronics Engineers) Transactions on Instrumentation and Measurement 40, n2 p360-365 Apr 91.

Keywords: Electric connectors, Transmission lines, Skin effect, Reprints, \*Thermal voltage converters, Thermal converters.

The RF-dc differences of thermal voltage converters (TVC's) caused by skin effect and transmission-line effects of different length input structures have been studied. Some discrepancies do exist between simple mathematical models and measured results for commonly used input connectors. The paper reports a study of these discrepancies and some worst-case results of changes in RF-dc difference due to connection and disconnection of TVC's.

PB91-236810 Not available NTIS National Inst. of Standards and Technology (NEL), Boulder, CO. Electromagnetic Technology Div. Excess Low-Frequency Flux Noise in dc Squids Incorporating Nb/Al-Oxide/Nb Josephson Junctions.

Final rept.

M. E. Huber, and M. W. Cromar. 1990, 2p Pub. in Physica B 165-166, p77-78 1990.

Keywords: \*SQUID devices, Electromagnetic noise, Josephson junctions, Direct current, Low frequency, Aluminum oxide, Niobium, Reprints, SIS(Superconductors).

The authors have fabricated thin-film dc SQUIDs (Superconducting QUantum Interference Devices) incorporating Nb/Al-Oxide/Nb tunnel junctions. The spectral density of the voltage noise, S(v), of stripline SQUIDs is characterized between 1 Hz and 2000 Hz. In this frequency range, S(v) is proportional to the square of the responsivity over a significant range of square of the responsivity over a significant range of bias conditions with an unusual frequency dependence. In a 7 pH SQUID, the spectral density of the flux noise, S(phi) at 1 Hz is less than 10 to the -11 power (Phi(0)) squared/Hz where Phi(0) is identically = h/2e. The observed noise does not appear to be environmental; also, it is independent of the value of the junction shunt resistance and whether the stripline material is a Pbin alloy or Nb. Subject to the constraint of a constant product of the junction area entited unrent constant product of the junction area, critical current density, and SQUID self-inductance in the SQUIDs studied, S(phi) is inversely proportional to the junction area.

100,737 PB91-236893 Not available NTIS National Inst. of Standards and Technology (EEEL), Gaithersburg, MD. Electricity Div. AC-DC Difference Relationships for Current Shunt

and Thermal Converter Combinations. Final rept.

J. R. Kinard, T. E. Lipe, and C. B. Childers. 1991, 4p See also PB91-101378.

Pub. in IEEE (Institute of Electrical and Electronics Engineers) Transactions on Instrumentation and Measurement 40, n2 p352-355 Apr 91.

Keywords: Alternating current, Direct current, Mutual inductance, Electrical measurement, Electric converters, Reprints, \*Thermal converters, Current shunts, Thermal voltage converters, Thermal current convert-

The paper describes the relationship between the overall ac-dc difference of a current-shunt/thermal-converter combination and the individual characteristics of the current shunt and thermal converter (TC) considered separately. Equations governing these characteristics are derived for the general case where the characteristics include mutual inductance between the shunt and the TC circuits, and for the simplified case such as the replacement of just a thermoelement (TE) within the TC, where the change in mutual inductance is negligible. Predicted and measured results are given for shunts used with different TC's.

100,738 PB91-237107 Not available NTIS National Inst. of Standards and Technology (EEEL), Gaithersburg, MD. Electricity Div.

New Low-Voltage Standards in the DC to 1-MHz Frequency Range.

Final rept.

N. M. Oldham, and R. M. Henderson. 1991, 5p

See also PB91-101493. Pub. in IEEE (Institute of Electrical and Electronics Engineers) Transactions on Instrumentation and Measurement 40, n2 p368-372 Apr 91.

Keywords: \*Standards, Electrical measurement, Audio frequencies, Radio frequencies, Low voltage, Potentiometers(Resistors), Electric potential, Dividers, Reprints, \*Voltage standards, Thermal voltage converters, Thermal converters.

Two new instruments for generating and measuring 1-200-mV signlas have been developed and used to test a number of different low-voltage measurement techniques. Differences between the various measurement methods at 100 mV are typically within + or - 20 ppm in the 1-20 kHz range and within + or - 300 ppm out to

100,739 PB91-237446 PB91-237446 Not available NTIS National Inst. of Standards and Technology (EEEL), Gaithersburg, MD. Electricity Div.

Improvements for Automating Voltage Calibrations Using a 10-V Josephson Array.

Final rept.

R. L. Steiner, and R. J. Astalos. 1991, 5p

See also PB91-101592. Pub. in IEEE (Institute of Electrical and Electronics Engineers) Transactions on Instrumentation and Measurement 40, n2 p321-325 Apr 91.

Keywords: \*Calibration, \*Standards, Josephson junctions, Direct current, Digital systems, Automation, Voltmeters, Reprints, \*Voltage standards, Josephson

A voltage standard system based on a 10-V Josephson array have been completely automated with three novel developments. First, a unique way of connecting Zener voltage standards, a digital voltmeter (DVM), and the array to a commercial standard cell scanner has provided necessary switching flexibility. Second, using a programmable millimeter wave attenuator has greatly simplified the selection of voltage steps. Third and last, programmed error checking, which verifies array steps by comparing measurement scatter to previously characterized system noise levels, has proven more reliable than visual observation. The operation of this new system is simplified enough for an inexpert user while the calibration uncertainty (1 sigma) is still a few parts in 100 million.

PB91-237586 Not available NTIS National Inst. of Standards and Technology (PL), Raithersburg, MD. Physics Lab. Office.

New International Electrical Reference Standards
Based on the Josephson and Quantum Hall Ef-

fects.

Final rept.

S. N. Taylor, and T. J. Witt. 1989, 16p Sponsored by Bureau International des Poids et Mesures, Sevres (France).

Pub. in Metrologia 26, n1 p47-62 1989.

Keywords: \*Electrical resistance, \*Voltage, \*Standards, Josephson effect, International, Reprints, \*Resistance standards, \*Voltage standards, Quantum Hall effect, Ohm, Volt.

The authors discuss the background and basis for the new international electrical reference standards of voltage and resistance that are to come into effect worldwide, starting on 1st January 1990. Founded on the Josephson and Quantum Hall effects, respectively, these new reference standards will improve significantly the international uniformity of electrical measurements and their consistency with the SI.

100.741

PB92-117076 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Electricity Div.

Need for Power Quality Testing Standards. Final rept.

Pillatept.
F. D. Martzloff. 1990, 2p
Pub. in Proceedings of National Conference Power
Quality for End-Use Applications (2nd), San Francisco,
CA., March 21-23, 1990, p171-172.

Keywords: \*Power supply circuits, \*Standards, \*Quality, \*Surges, Voltage regulation, Power measurement, Electronic equipment, Power, Voltage regulators, Overvoltage, Overcurrent, Reprints.

The quality of the power supplied to sensitive electronic equipment is an important issue. Quantifying this quality, however, is difficult under the present state of nonexistent or uncoordinated standards. Improvements in the situation described as poor power quality can be achieved by reducing the sensitivity of equipment to power line disturbances, or by limiting the injection of disturbances. While these remedies might seem obvious in principle, their implementation appears more difficult. Voluntary standards provide a guide for such an implementation. The formation by IEEE of a Standards Coordinating Committee on Power Quality responds to the need.

100.742

PB92-117431 Not available NTIS National Inst. of Standards and Technology (EEEL), Gaithersburg, MD. Electricity Div.

Performance Evaluation of a New Audio-Frequencv Power Bridge.

Final rept.

B. C. Waltrip, and N. M. Oldham. 1991, 4p

See also PB91-101634.
Pub. in IEEE (Institute for Electrical and Electronics Engineers) Transactions on Instrumentation and Measurement 40, n2 p380-383 Apr 91.

Keywords: \*Electric bridges, Electrical measurement, Alternating current, Audio frequencies, Power factor, Electrical impedance, Performance evaluation, Wattmeters, Reprints.

Several techniques for measuring active and reactive power in the 50 Hz to 20 kHz frequency range are described. The approaches include: (1) the development of a high-precision sampling wattmeter using a resistive attenuator, a shunt, and two commercially available sampling voltmeters configured as a dual-channel equivalent-time sampler; (2) the development of another high-precision sampling wattmeter using the same shunt and attenuator, a high-impedance, wideband differential amplifier, and a commercially available, dual-channel, direct-sampling waveform analyzer; (3) for zero power factor measurements, the use of a digital generator to produce precise phase shifts from + pi/2 to pi/2; and (4) the use of simultaneous thermal voltage and current measurements for unity power factor measurements. These approaches were developed to evaluate a new high-accuracy, audio-frequency power bridge that is based on ac voltage and impedance measurements.

### **Electromechanical Devices**

100.743

PB91-236620 Not available NTIS National Inst. of Standards and Technology (EEEL), Boulder, CO. Electromagnetic Fields Div. Determining Adapter Efficiency by Envelope Averaging Swept Frequency Reflection Data.

W. C. Daywitt. 1990, 5p Pub. in IEEE (Institute of Electrical and Electronics Engineers) Transactions on Microwave Theory and Techniques 38, n11 p1748-1752 Nov 90.

Keywords: \*Adapters, Electric connectors, Microwave equipment, Millimeter waves, Metrology, Efficiency, Reprints, Automated network analyzers.

A simple automated network analyzer swept frequency technique for measuring adapter efficiency across its entire frequency band is described. Envelope averaging is used to avoid the model assumptions usually found in regression averaging techniques. Calculations show that errors arising from the theoretical assumptions leading to the technique are around 0.004 dB for a common WR 42 waveguide-to-coaxial adapt-

### **Optoelectronic Devices & Systems**

100.744

AD-A227 836/4 PC A01/MF A01 National Inst. of Standards and Technology, Gaithers-

Photomultiplier Housing for Vacuum Operation of Side-on 1P28-Type Tubes.

W. Braun, R. Klein, A. Fahr, and A. Mele. 1990, 4p ARO-25911.3-CH.

Contract MIPR-ARO-119-89

Pub. in Review of Scientific Instruments, v61 n5 p1558-1560 May 90.

Keywords: \*Housings, Operation, Photometry, \*Photomultiplier tubes, Reprints, Sides, Tubes, Vacuum, Vacuum ultraviolet radiation.

A design for the mounting of a side-on tube such as the 1P28 type which has proven simple to construct, reliable, and evacuatable is described. Keywords: Reprints; Housing; Photomultiplier; Vacuum Ultraviolet; photometry; design. (jhd)

100.745

PB91-134734 Not available NTIS National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div.

Progress in the Development of Miniature Optical Fiber Current Sensors.

Final rept.

D. Tang, and G. W. Day. 1988, 1p Sponsored by Defense Nuclear Agency, Washington, DC., and Los Alamos National Lab., NM.

Pub. in Proceedings of IEEE (Institute of Electrical and

Electronics Engineers) Lasers and Electro-Optics Society 1988 LEOS Annual Meeting, Santa Clara, CA., November 2-4, 1988, p306.

Keywords: \*Electric current meters, \*Fiber optics, Faraday effect, Birefringence, Optical measuring instru-ments, Reprints, \*Optoelectronic devices, \*Optical fibers, Sensors.

Recent improvements in fiber annealing technology have allowed the authors to substantially reduce the size and increase the number of turns of fiber current sensing coils. Coils as small as 7 mm diameter have been successfully annealed. Coils with more than 100 turns and diameters of 1 or 3 cm are routinely produced. The linear birefringence of such coils is small enough that Faraday rotation is not measurably diminished. Increased loss as a result of annealing is minimal.

100,746

PB91-134742 Not available NTIS National Inst. of Standards and Technology (NEL), Boulder, CO. Electromagnetic Technology Div Practical Considerations in the Design of Optical Fiber Current Sensors.

Final rept. D. Tang, A. H. Rose, and G. W. Day. 1990, 6p Sponsored by National Aeronautics and Space Administration, Washington, DC., Department of Defense, Washington, DC., and Department of Energy, Washington, DC.

# **Optoelectronic Devices & Systems**

Pub. in Proceedings of International Congress on Optical Science and Engineering, The Hague, Netherlands, March 12-15, 1990, 6p.

Keywords: \*Electric current meters, \*Fiber optics, Optical measuring instruments, Birefringence, Reprints, \*Optoelectronic devices, \*Optical fibers, Sensors.

While current sensors based on the Faraday effect in bulk materials have shown good success in field tests, the use of single mode fiber as the sensing element has both technical and economic advantages. In the paper the authors describe some of the practical prob-lems that have inhibited the development of fiber current sensors. Recent research suggests that most of these problems, including especially the problem of linear birefringence in the sensing coils, can be solved. Instruments providing a measurement quality approaching that set by fundamental material parameters can now be achieved.

100 747

PB91-148254 Not available NTIS National Bureau of Standards (ICST), Gaithersburg,

MD. Advanced Systems Div.
Conformance Verification of FDDI Stations.

Final rept.

L. Zuqiu, and W. E. Burr. 1988, 15p

Pub. in Fiber and Integrated Optics 7, n3 p181-195 1988.

Keywords: \*Local area networks, Fiber optics, Verification, Standards, Tests, Reprints, \*FDDI(Fiber Distributed Data Interface), \*Fiber distributed data interface, \*Token ring networks.

The Fiber Distributed Data Interface (FDDI) is an emerging standard for a 100 Mbit/s. fiber optic token ring Local Area Network. The paper outlines an approach to testing FDDI stations to verify their conformance to the FDDI standards.

100.748

PB91-148999 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Semiconductor Electronics Div. Micromachined Thermal Radiation Emitter from a Commercial CMOS Process.

Final rept. M. Parameswaran, A. M. Robinson, D. L. Blackburn,

M. Gaitan, and J. Geist. 1991, 3p Pub. in IEEE (Institute of Electrical and Electronics Engineers) Electron Device Letters 12, n2 p57-59 Feb 91.

Keywords: \*Infrared sources, \*Thermal radiation, CMOS, Reprints, Thermal scene simulation.

Fabrication of thermally isolated micromechanical structures capable of generating thermal radiation for dynamic thermal scene simulation (DTSS) is described. Complete compatibility with a commercial CMOS process is achieved through design of a novel, but acceptable, layout for implementation by the CMOS foundry using its regular process sequence. Following commercial production and delivery of the CMOS chips, a single maskless etch in an aqueous ethylenediamine-pyrocatechol mixture (EDP) is performed to realize the micromechanical structures. The resulting structures are suspended plates consisting of polysilicon resistors encapsulated in the field and CVD oxides available in the CMOS process. The plates are suspended by aluminum heater leads that are also encaps capsulated in the field and CVD oxides. Studies of the suitability of these structures for DTSS have been initiated, and early favorable results are reported.

PB91-149146 Not available NTIS
National Inst. of Standards and Technology (NEL), Boulder, CO. Electromagnetic Technology Div Performance and Limitations of Faraday Effect Sensors.

Final rept.

A. H. Rose, M. N. Deeter, D. Tang, and G. W. Day. 1990, 1p

1990, 1p Sponsored by Department of Energy, Washington, DC., and Department of Defense, Washington, DC. Pub. in Proceedings of Electrochemical Society Fall Meeting, Seattle, WA., October 14-19, 1990, p1093.

Keywords: \*Optical measuring instruments, \*Electric current meters, \*Magnetic fields, \*Faraday effect, Measurement, Sensors, Reprints.

Sensors that use the Faraday effect to measure electric current and magnetic fields are becoming more prevalent because of their sensitivity, bandwidth, stability, and ability to operate in the presence of high voltage or EMI. They are now routinely used to measure large current pulses and are becoming available to the power industry. They can measure currents from milliamperes to megamperes and magnetic fields in the nanotesla range. Their size has been reduced and stability increased. Their speed is limited by material effects or transit time, but often extends to hundreds of megahertz.

100.750 PB91-162206 Not available NTIS National Inst. of Standards and Technology (NEL), Boulder, CO. Electromagnetic Fields Div. Photonic Probes for the Measurement of Electro-

magnetic Fields Over Broad Bandwidths. Final rept.

K. D. Masterson, L. D. Driver, and M. Kanda. 1989,

Pub. in Proceedings of IEEE (Institute of Electrical and Electronics Engineers) National Symposium on Electromagnetic Compatibility, Denver, CO., May 23-25, 1989, p1-6.

Keywords: \*Photonics, Electromagnetic fields, Directional couplers, Pockels cell, Fiber optics, Sensors, Reprints. \*Electric field meters. Optical modulators.

The characteristics of photonic systems which make them especially well suited for use as broadband electromagnetic field sensors are discussed. Transfer functions are given for the individual components of such a measurement system, with special emphasis given to those of Pockels-cell and modified-directional-coupler optical modulators. An isotropic electricfield meter having 15 cm resistively tapered dipole elements combined with bulk crystal, Pockels-cell modulators is described. The meter's frequency response is flat between 30 kHz and 100 MHz, except for resonances in the modulator crystals that occur between 1 and 10 MHz. A photonic probe that uses a modified directional-coupler modulator is also briefly described.

100,751 PB91-174615 Not available NTIS
National Inst. of Standards and Technology (NEL),
Boulder, CO. Electromagnetic Technology Div.
Iron-Garnet Magnetic Field Sensors with 100 pT/
per square root Hz Noise-Equivalent Field.
Final rept

M. N. Deeter, A. H. Rose, and G. W. Day. 1990, 4p Pub. in Proceedings of Optical Fibre Sensors Confer-ence, Sydney, New South Wales, Australia, December 2-6, 1990, p341-344.

Keywords: \*Magnetic detection, \*Fiber optics, Yttrium iron garnets, Faraday effect, Magnetic fields, Magnetooptics, Substitutes, Gallium, Sensors, Reprints.

The sensitivity of Faraday-effect sensors incorporating diamagnetically substituted yttrium iron garnet (YIG) is potentially much higher than of sensors employing pure YIG. Results of Faraday rotation linearity and sensitivity measurements are presented for gallium-substi-tuted YIG. At 500 Hz, the noise-equivalent magnetic field is approximately 100 pT/square root of Hz.

100,752 PB91-174706 PB91-174706 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Radiometric Physics Div.

Electronic and Radiometric Characteristics of

Near Infrared Photodiodes. Final rept.

G. Eppeldauer, M. Tsudagawa, E. Zalewski, and J. Houston. 1987, 10p Pub. in Proceedings of International Symposium on

Tech. Comm. Photon Detect., Int. Meas. Confed., v13 p215-224 1987.

Keywords: \*Photodiodes, \*Radiometry, Near infrared radiation, Quantum efficiency, Indium phosphides, Reprints, Gallium indium arsenides.

Three different types of infrared photodiodes from three manufacturers have been examined for their electronic and radiometric performance. Measure-ments were made of the shunt resistance, absolute re-sponse, reflectance, uniformity and linearity. The results of these measurements are presented in a manner that selects the best device for radiometric applications. From the limited sampling of devices available at the time of the study, InGaAs/InP photodiodes appear to be the most suitable. They have a very high internal quantum efficiency, are linear and reasonably

uniform, and may be expected to perform well in high gain applications. Their high internal quantum efficiency can be interpreted as indicating that they may be suitable for self-calibration in a manner resembling silicon photodiodes.

100,753

PB91-175109 Not available NTIS National Inst. of Standards and Technology (NEL), Boulder, CO. Electromagnetic Fields Div. Optical Fiber Current Sensors with Temperature

Stabilities Near the Material Limit. Final rept.

D. Tang, A. H. Rose, and G. W. Day. 1990, 4p Pub. in Proceedings of Optical Fibre Sensors Confer-ence (7th), Sydney, New South Wales, Australia, De-cember 2-6, 1990, p77-80.

Keywords: \*Electric current meters, \*Optical fibers, Thermal stability, Faraday effect, Sensors, Reprints.

The authors describe an optical fiber current sensor with a normalized temperature coefficient of +0.000084/K over the range from -75 to +145C. This is within 20% of the limit set by the temperature dependence of the Verdet constant measured in bulk silica. Packaging of the sensor coil degrades its stability, but a fully packaged coil with a stability of  $\pm 0.00017/K$  over the range from -30 to  $\pm 125C$  has also been demonstrated.

100,754

PB91-175158 Not available NTIS National Inst. of Standards and Technology (NEL), Boulder, CO. Electromagnetic Technology Div. Faraday Effect Current Sensing Using a Sagnac Interferometer with a 3x3 Coupler. Final rept.

L. R. Veeser, and G. W. Day. 1990, 189p Pub. in Proceedings of Optical Fibre Sensors Conference (7th), Sydney, New South Wales, Australia, December 2-6, 1990, p325-328.

Keywords: \*Optical measuring instruments, \*Electric current meters, \*Fiber optics, Optical interferometers, Sagnac effect, Faraday effect, Sensors, Reprints, Optical couplers.

The authors demonstrate a fiber optic current sensor based on a Sagnac interferometer with a 3x3 fiber cou-pler. Compared to the more common Sagnac interferometer with a 2x2 coupler, the design offers the additional benefits of a greater response for small signals and the unambiguous interpretation of signals that exceed the period of the response function.

100.755

PB91-187625

(Order as PB91-187617, PC A06/MF A01) National Inst. of Standards and Technology, Gaithersburg, MD.

Linearity of a Silicon Photodiode at 30 MHz and Its Effect on Heterodyne Measurements.

A. L. Migdall, and C. Winnewissser. 1991, 4p Included in Jnl. of Research of the National Institute of Standards and Technology, v96 n2 p143-146 Mar/Apr

Keywords: \*Photodiodes, Si semiconductor detectors, Silicon diodes, Light modulation, Laser radiation, High frequency, Heterodyning, Irradiance, Linearity.

The effect of optical irradiance on the linearity of a Si photodiode was studied. These results are compared for light modulated at 30 MHz and at dc as the optical irradiance was varied over a 9 decade range. The authors discuss how these results affect the use of the detector as a heterodyne receiver. As the optical irradiance varied from 0.01 to .1000 mW/sq cm, while mainance varied from 0.01 to .1000 mw/sq cm, while maintaining constant total power, the photocurrent was constant to about 1%, but as the power density increased further, the photocurrent increased about 13%. At the highest densities that the authors could achieve, about 60 million mW/sq cm, there was only slight evidence of the onset of saturation. These results are of importance in the work to use optical heterodyne detection to measure filter transmittances over a wide dynamic range. The results provide guidelines for achieving maximum accuracy when using this particular diode as an optical heterodyne receiver.

100,756

PB91-194845

Not available NTIS

# Optoelectronic Devices & Systems

National Inst. of Standards and Technology (NEL), Boulder, CO. Electromagnetic Technology Div.
Hydrogenated Amorphous Germanium Detectors
Deposited onto Channel Waveguides.

Final rept.

D. R. Larson, and R. J. Phelan. 1990, 3p Pub. in Optics Letters 15, n10 p544-546, 15 May 90.

Keywords: \*Ge semiconductor detectors, \*Photodetectors, Amorphous materials, Integrated optics, Lithi-um niobates, Picosecond pulses, Subtrates, Glass, Doped materials, Phosphorus, Reprints.

The authors have fabricated hydrogenated amorphous germanium photodetectors coupled to channel waveguides in glass and lithium niobate substrates. They measured a pulse response duration of 140 psec (FWHM), which is shorter than that of any previously reported photodetectors deposited onto dielectric waveguides. The optical gap, which determines the spectral response characteristics, is approximately 1.2 eV. A photoconductive gain of 18 was measured in phosphorus-doped detectors.

100,757 PB91-203349 Not available NTIS National Bureau of Standards (NML), Gaithersburg,

MD. Radiation Physics Div.
Stable, High Quantum Efficiency Silicon Photodiodes for Vacuum-UV Applications.

R. Korde, L. R. Canfield, and B. Wallis. 1988, 8p
Pub. in Proceedings of SPIE (Society of Photo-Optical
Instrumentation Engineers) Ultraviolet Technology II, Orlando, FL., April 4-5, 1988, p153-160.

\*Ultraviolet detectors, \*Photodiodes. Vacuum ultraviolet radiation, Silicon diodes, Quantum efficiency, Radiometry, Standards, Reprints.

Silicon photodiodes have been developed by defectfree phosphorus diffusion having practically no carrier recombination at the Si-SiO2 interface or in the front diffused region. The quantum efficiency of these photodiodes was found to be around 120% at 100 nm. Unlike the previously tested silicon photodiodes, the developed photodiodes exhibit extremely stable quantum efficiency over extended periods of time. Currently, the authors are investigating the possibility of using these photodiodes as vacuum ultraviolet detector standards.

100,758 PB91-203976 PB91-203976 Not available NTIS National Inst. of Standards and Technology (NEL), Boulder, CO. Electromagnetic Technology Div. Integrated-Optic Waveguide Glass Lasers.

N. A. Sanford, K. J. Malone, and D. R. Larson. 1991,

1p Pub. in Proceedings of Optical Fiber Communication Conference, San Diego, CA., February 18-22, 1991,

Keywords: \*Integrated optics, \*Waveguide lasers, Mode locked lasers, Q switched lasers, Glass lasers, Rare earth elements, Doped materials, Chemical vapor deposition, Reprints.

Rare-earth-doped integrated-optic waveguide devices offer new miniaturized cw and pulsed lasers, amplifiers, and other active elements. Fabrication methods which use bulk glasses as well as chemical-vapor deposition techniques are being explored.

100,759 PB91-204131

Final rept.

Not available NTIS National Inst. of Standards and Technology (NEL), Boulder, CO. Electromagnetic Technology Div.
Analyzing Integrated Optical Waveguides: A Comparison of Two New Methods.

Final rept. Y. Tu, I. C. Goyal, and R. L. Gallawa. 1990, 3p Pub. in Applied Optics 29, n36, p5313-5315, 20 Dec

Keywords: \*Optical waveguides, \*Integrated optics, WKB approximation, Fourier series, Numerical analysis, Comparison, Reprints.

The authors present a comparison of two recently developed methods of analyzing optical waveguides. One of them is numerical, and the other is an approximate analytical method.

100,760 PB91-236901

Not available NTIS

National Inst. of Standards and Technology (EEEL), Gaithersburg, MD. Semiconductor Electronics Div. Generalized Photodiode Self-Calibration Formula. Final rept.

R. Kohler, J. Geist, and J. Bonhoure, 1991, 3p Pub. in Applied Optics 30, n7 p884-886, 1 Mar 91.

Keywords: \*Photodiodes, \*Calibration, Quantum efficiency, Silicon diodes, Reprints, Self calibration, Oxide bias experiment, Reverse bias experiment.

The authors have derived the photodiode self-calibration formula for calculating the internal quantum effi-ciency of silicon photodiodes from the results of one, two, or three independent self-calibration experiments and from the results of ozide bias and reverse bias experiments in conjunction with a calculation of the effect of Auger recombination. They show that the formula published elsewhere for these three effects is not correct

100.761

PB91-237792 Not available NTIS National Inst. of Standards and Technology (EEEL), Gaithersburg, MD. Electronics and Electrical Engineering Lab. Office.

Dealing with Obvious Issues in Lighting.

J. A. Worthey. 1991, 4p Pub. in Lighting Design and Application 21, n8 p15, 17-19, Aug 91.

Keywords: \*Illuminating, \*Daylighting, Research management, Design criteria, Luminance, Light sources, Lighting systems, Color, Reprints.

An early 'controlled study' of lighting effects is reviewed. Although the authors did not present it in that way, the study controlled for most obvious differences between two light sources, then looked for possible effects of more subtle physical differences. The outcome was null -- no difference in the light sources. The suggestion is made that while subtle differences may be easier to study in a simple experiment, obvious differences may be more important. To deal with obvious facts, an approach involving more theory and calculation is appropriate.

PC A05/MF A02 PB92-110261 National Inst. of Standards and Technology, Gaithers-

Journal of Research of the National Institute of Standards and Technology. July-August 1991. Volume 96. Number 4.

c1991, 100p

Also available from Supt. of Docs as SN703-027-0041-5. See also PB92-110279 through PB92-110311 and PB91-216705. Library of Congress catalog card no.

Keywords: \*Photodiodes, \*Computerized simulation, Antenna radiation patterns, Building fires, Room fires.

Contents:

General Analytic Correction for Probe-Position Errors in Spherical Near-Field Measurements; Data for Room Fire Model Comparisons; Numerical Modeling of Silicon Photodiodes for High-Accuracy Applications--Part I. Simulation Programs;

Numerical Modeling of Silicon Photodiodes for High-Accuracy Applications--Part II. Interpreting Oxide-Bias Experiments;

Numerical Modeling of Silicon Photodiodes for High-Accuracy Applications—Part III. Interpolating and Extrapolating Internal Quantum-Efficiency Calibrations.

100,763 PB92-110295

(Order as PB92-110261, PC A05/MF A01) National Inst. of Standards and Technology, Gaithersburg, MD.

Numerical Modeling of Silicon Photodiodes for High-Accuracy Applications. Part 1. Simulation Programs.

J. Geist, D. Chandler-Horowitz, A. M. Robinson, and C. R. James. c1991, 7p
Prepared in cooperation with Alberta Univ.. Edmonton.

Included in Jnl. of Research of the National Institute of Standards and Technology, v96 n4 p463-469 Jul/Aug

Keywords: \*Photodiodes, \*Computerized simulation, Mathematical models, Silicon diodes, Quantum efficiency, One dimensional, Accuracy, PC-1D computer program.

The suitability of the semiconductor-device modeling program PC-1D for high-accuracy simulation of silicon photodiodes is discussed. A set of user interface programs optimized to support high-accuracy batch-mode operation of PC-1D for modeling the internal quantum efficiency of photodiodes is also described. The optimization includes correction for the dark current under reverse- and forward-bias conditions before calculating the quantum efficiency, and easy access to the highest numerical accuracy available from PC-1D, neither of which is conveniently available with PC-1D's standard user interface.

100.764

PB92-110303

(Order as PB92-110261, PC A05/MF 01) National Inst. of Standards and Technology, Gaithersburg, MD.

Numerical Modeling of Silicon Photodiodes for High-Accuracy Applications. Part 2. Interpreting Oxide-bias Experiments.

J. Geist, R. Koehler, R. Goebel, A. M. Robinson, and C. R. James. c1991, 9p

Prepared in cooperation with Bureau International des Poids et Mesures, Sevres (France), and Alberta Univ., Edmonton.

Included in Jnl. of Research of the National Institute of Standards and Technology, v96 n4 p471-479 Jul/Aug

Keywords: \*Photodiodes, \*Computerized simulation, Silicon diodes, Quantum efficiency, Mathematical models, Numerical solution, Visible radiation, PC-1D computer program, Oxide bias experiments.

The semiconductor device modeling program PC-1D and the programs that support its use in high-accuracy modeling of photodiodes, all of which were described in Part I of the series of papers, are used to simulate oxide-bias self-calibration experiments on three different types of silicon photodiodes. It is shown that these simulations can be used to determine photodiode characteristics, including the internal quantum efficiency for the different types of photodiodes. In the latter case, the simulations provide more accurate values than can be determined by using the conventional data reduction procedure, and an uncertainty estimate can be derived. Finally, it is shown that 0.9997 + or - is a nominal value for the internal quantum efficiency of one type of photodiode over the 440 to 460 nm spectral region.

100,765

PB92-110311

(Order as PB92-110261, PC A05/MF A01) National Inst. of Standards and Technology, Gaithersburg, MD.

Numerical Modeling of Silicon Photodiodes for High-Accuracy Applications. Part 3. Interpolating and Extrapolating Internal Quantum-Efficiency Calibrations.

J. Geist, A. M. Robinson, and C. R. James. c1991,

Prepared in cooperation with Alberta Univ., Edmonton. Included in Jnl. of Research of the National Institute of Standards and Technology, v96 n4 p481-492 Jul/Aug

Keywords: \*Photodiodes, \*Computerized simulation, Silicon diodes, Mathematical models, Quantum efficiency, Visible radiation, Near infrared radiation, Interpolation, Extrapolation, PC-1D computer program.

The semiconductor device modeling program PC-1D and the programs that support its use in high-accuracy modeling of photodiodes, all of which were described in Part I of the series of papers, are used to simulate the interpolation of high-accuracy calibrations in the spectral region between 450 nm and 850 nm. Convenient interpolation formulae that depend only upon wavelength are derived. Uncertainty spectra for a number of sources of error are also derived. The formulae are normalized to experimental internal-quantum efficiency calibrations in the 440 to 470 nm spectral region and at 860 nm and are used to interpolate the calibration values between these wavelengths. The results of the interpolations are compared with experimental calibration data that are available at a few wavelengths between 440 and 860 nm.

# **Optoelectronic Devices & Systems**

100,766 PB92-112382 PC A05/MF A02 National Inst. of Standards and Technology, Gaithersburg, MD.
HaCdTe Detector Reliability Study for the GOES

Program.

D. G. Seiler, G. G. Harman, J. R. Lowney, S. Mayo, and W. S. Liggett. Sep 91, 100p NISTIR-4687 Sponsored by National Oceanic and Atmospheric Administration, Rockville, MD.

Keywords: \*GOES satellites, \*Infrared detectors, Intermediate infrared radiation, Mercury cadmium tellur-Satellite-borne instruments. Reliability(Electronics), Degradation.

The report summarizes the results of a special assessment concerning the reliability of certain infrared detectors for the Geostationary Operational Environmental Satellite (GOES) system. The data made available by ITT on detector resistances and signals support the conclusion that degradation of some detector re-sponses has occurred, even when the estimated measurement uncertainty is included. Statistical analysis of the 11-micrometer detectors confirmed that detector 11-105 decreased in signal with time. The existing data available to NIST is not sufficient to identify uniquely the cause of degradation or unstable behavior present in a number of detectors. NIST's physical examination of several detectors by optical and SEM microscopy methods and an examination and analysis of the Detector Measurement Database has yielded several plausible possible mechanisms for the ob-served degradation. The possible mechanisms are related to the detector fabrication or processing steps and include: Incomplete or poor passivation procedures, excess mercury diffusion resulting from the ionbeam milling fabrication step, poor indium electrical contacts produced by the indium-plated fabrication step, and delamination of the ZnS antireflection optical coating. Other observed problems are also discussed.

PB92-116763 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Radiometric Physics Div. Temperature Monitored/Controlled Silicon Photodiodes for Standardization.

Final rept.

Final rept.

G. Eppeldauer. 1991, 7p

Pub. in Proceedings of SPIE (Society of Photo-Optical Instrumentation Engineers) - Surveillance Technologies, v1479 p71-77 1991.

Keywords: \*Photometers, \*Radiometers, Silicon diodes, Temperature measurement, Temperature control, Standardization, Photodiodes, Correction, Re-

Two alternative approaches to reducing errors in radiometers and photometers caused by temperature variations involve temperature monitoring and temperature control. In the first method, the measurement results are interpreted using the temperature of the detector at the time of measurement. The other method is to control the temperature of the detector to a constant value. Design considerations and examples of both approaches are discussed.

100.768 PB92-116771 Not available NTIS National Inst. of Standards and Technology (NML), Fourteen-Decade Photocurrent Measurements with Large-Area Silicon Photodiodes at Room

Temperature. Final rept.

G. Eppeldauer, and J. E. Hardis. 1991, 9p Pub. in Applied Optics 30, n22 p3091-3099, 1 Aug 91.

Keywords: \*Optical detectors, \*Photodiodes, \*Photocurrents, Electrical measurement, Silicon diodes, Room temperature, Radiometry, Bandwidth, Sensitivitv. Reprints.

Recent improvements in commercial silicon photo-diodes and operational amplifiers permit electrical noise to be reduced to an equivalent of 0.1 fA of photocurrent when a measurement time of 400 s is used. This is equivalent to a photocurrent resulting from fewer than 800 photons/s, and it implies a dynamic range of 14 orders of magnitude for a detector circuit. The authors explain the circuit theory, paying particular attention to the measurement bandwidth, the causes of noise and drift, and the proper selection of circuit components. These optical radiation detectors complement the primary radiometric standards. These detectors may replace photomultiplier tubes that have been used traditionally and or that were too costly to be used.

### **Power & Signal Transmission Devices**

100,769 PB91-133892 PB91-133892 Not available NTIS
National Inst. of Standards and Technology (NEL),
Boulder, CO. Electromagnetic Technology Div.
AC Loss Measurements of Two Multifilamentary
Noticempagite Strends NbTi Composite Strands.

NBTI Composite Stratus. Final rept. E. W. Collings, K. R. Marken, M. D. Sumption, R. B. Goldfarb, and R. J. Loughran. 1990, 8p See also DE90005388. Sponsored by Department of Energy, Washington, DC. Div. of High Energy Physics. Pub. in Advances in Cryogenic Engineering (Materials) 26, p.160-176 1990. 36, p169-176 1990.

Keywords: Filament winding, Magnetization, Hysteresis, Reprints, \*Superconducting wires, \*AC losses, Niobjum titanium.

As part of an interlaboratory comparative testing program conducted in support of the Versailles Agreement on Advanced Materials and Standards (VAMAS), transversefield DC hysteresis loss measurements were made at liquid-helium temperatures at fields of up were made at liquid-riellorif temperatures at leids of vides of 3 T (30 kG) on two samples of multifilamentary NbTi composite. The strands differed widely in filament number, were comparable in filament diameter, and one of them was provided with a Cu-Ni barrier between the filaments. The results have been analyzed, and magnetically deduced critical current density values obtained (for comparison with directly measured trans port data) using various standard techniques. Based on these studies, a figure-of-merit for AC loss is recommended. The Cu-matrix strand, with its interfilamentary spacing of less than 1 micrometer, exhibited pro-nounced proximity-effect-induced coupling losses; this was not observed in the mixed-matrix strand which possessed not only a Cu-Ni barrier but also an interfilamentary spacing of typically 4 micrometers.

PB91-134114 Not available NTIS National Inst. of Standards and Technology (NEL), Boulder, CO. Electromagnetic Fields Div. Determination of Scattering Parameters with Respect to the Characteristic Impedance of Precision Coaxial Air-Line Standards.

Coaxia An-Line Statistics
Final rept.
D. R. Holt. 1990, 2p
Pub. in Proceedings of Conference on Precision Electromagnetic Measurements (CPEM 90), Ottawa, Canada, June 11-14, 1990, p282-283.

Keywords: \*Coaxial cables, Characteristic impedance, Skin effect, Surface roughness, Scattering, Standards, Reprints.

Scattering parameter expressions with respect to the characteristic impedances in correspondence to the principal mode are developed for the coaxial air-line standard. Dimensional variations of the inner and outer conductors and skin effect loss are included in the model. The local characteristic impedance, which is found from the stored energy principle, is derived from the forward and backward voltage and current waves of the principal mode. Four sources of error for absolute value of S (sub 11) are discussed.

PB91-134650 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Electricity Div. Partial Discharges in Low Voltage Cables. Final rept. 100,771 PB91-134650

Final rept.

J. P. Steiner, and F. D. Martzloff. 1990, 4p

Pub. in Proceedings of IEEE (Institute of Electrical and
Electronics Engineers) International Symposium on
Electrical Insulation, Toronto, Canada, June 3-6, 1990,

Keywords: \*Electrical insulation, \*Electric discharges, Signal processing, Reprints, \*Electric cables, Low voltage, Test methods.

Testing of high voltage apparatus for partial discharges has long been recognized as an important

part of quality control for these devices. Recently, interest has been focused on methods for testing low voltage cables to determine their integrity under ad-verse operating conditions such as a loss of coolant accident. A new method using partial discharges, is presented which has the potential for locating breaches in the insulation of in situ, low voltage, multiconductor cables.

100,772

PB91-134759 Not available NTIS National Inst. of Standards and Technology (NEL), Boulder, CO. Electromagnetic Technology Div. Magnetoresistance of Multifilament AI/AI-Alloy Conductors. Final rept.

C. A. Thompson, and F. R. Fickett. 1990, 7p Pub. in Advances in Cryogenic Engineering Materials, v36 p663-669 1990.

Keywords: \*Electric conductors, Aluminum alloys, Reprints, \*Magnetoresistance, Multifilaments.

Previously the authors have shown that composite monofilament conductors consisting of very pure aluminum confined in an Al-Fe-Ce alloy sheath show an anomalously high magnetoresistance compared to pure aluminum. Some monofilament conductors showed values of Delta R/R in excess of 50 at 4 K in fields of 10 T, whereas pure aluminum values are usually an order of magnitude smaller. Concerns that similar anomalous behavior might occur in multifilament wires of the same materials prompted this study. Multifilamentary conductors with pure aluminum filaments contained in an AI-Fe-Ce matrix have been investigat-

100,773

Not available NTIS PB91-161943 National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Polymers Div. Proceedings of Cable '89 Workshop.

Final rept.

M. G. Broadhurst, and E. Kelly. 1990, 119p Pub. in Proceedings of JICABLE/EPRI/CEA Work-shop 'Cable 89' The Aging of Extruded Dielectric Cables, St. Petersburg, FL., November 2-3, 1990, 119p.

Keywords: \*Meetings, \*Polymers, \*Electric cables, \*Dielectric materials, Power lines, Extrusion, Aging tests, Maintenance, Performance prediction, Acceler-ated tests, Electrical insulators, Reprints.

The report presents the proceedings of the workshop 'Cable 89' on The Aging of Extruded Dielectric Cables. The workshop was held in St. Petersburg, FL on November 2-3, 1989. The sponsoring organizations are The Electric Power Research Institute (US), the Canadian Electric Association and JICABLE (France). Attendance at the workshop was by invitation only, and attendees included 60 representatives of universities, research organizations, electric utilities, and manufac-turers of insulating polymers and power cables, from eight countries. The workshop was created as a forum for world experts to relate and compare their service experiences, theoretical, fundamental and experimental studies, and test results on the topic of aging of solid dielectric cables. The overall topic included materials aging, cable and accessories aging, diagnostic tests, accelerated aging and service experiences and conditions. The first half day of the workshop featured six overview presentations by international experts. The presentations and the brief discussions that followed each presentation are included in the report. The second half day was devoted to discussions within three separate working groups dealing with the three topic areas: materials, cables, and accelerated tests. Reports from the three working groups were given on the third half day, and are included in the report with the general discussions that followed each one.

100,774

PB91-236752 Not available NTIS National Inst. of Standards and Technology (EEEL), Boulder, CO. Electromagnetic Technology Div. Methods of Analyzing Planar Optical Waveguides. Final rept. I. C. Goyal, R. L. Gallawa, and A. K. Ghatak. 1991,

Pub. in Optic Letters 16, n1 p30-32, 1 Jan 91.

# **Power & Signal Transmission Devices**

Keywords: \*Optical waveguides, \*Optical fibers, \*Fiber optics, Wave equations, Integrated optics, WKB approximation, Reprints.

The authors present a new approximate solution of the scalar-wave equation for planar optical waveguides with arbitrary refractive-index profiles. Test calculations are done for an index profile with a known solu-tion. The comparison demonstrates the accuracy of their method. The method may also be applied to circularly symmetric optical fibers.

100,775 PB91-236992 Not available NTIS National Inst. of Standards and Technology (EEEL), Boulder, CO. Electromagnetic Fields Div. Characteristic Impedance Determination Using

Propagation Constant Measurement. Final rept.

R. Marks, and D. Williams. 1991, 3p
Pub. in IEEE (Institute of Electrical and Electronics Engineers) Microwave and Guided Wave Letters 1, n6 p141-143 Jun 91.

Keywords: \*Transmission lines, \*Characteristic impedance, Electrical conductivity, Electrical measurement, Reprints, Microwave monolithic integrated circuits, Coplanar waveguides.

A method is demonstrated where by the characteristic impedance of transmission lines may be easily determined from a measurement of the propagation constant. The method is based on a rigorous analysis using realistic approximations to account for the effects of imperfect conductors. Numerical studies indicate that high accuracy is possible, and experiments using coplanar waveguide demonstrate the advantage of the method in the interpretation of S-parameters.

100.776 PB92-116656 Not available NTIS National Inst. of Standards and Technology (EEEL), Boulder, CO. Electromagnetic Fields Div. Mode-Stirred Chamber for Measuring Shielding Effectiveness of Cables and Connectors: Assessing MIL-STD-1344A Method 3008.

Final rept. M. L. Crawford, and J. M. Ladbury. 1989, 7p See also PB89-149264.

Pub. in Connection Technology 5, n6 p45-51 Jun 89.

Keywords: \*Electromagnetic shielding, \*Electric connectors, \*Electric cables, Communication cables, Ultrahigh frequency, Superhigh frequency, Electrical measurement, Recommendations, Reprints, Mode stirred method.

The mode-stirred method for measuring the shielding effectiveness (SE) of cables and connectors as specified in MIL-STD-1344A Method 3008 is examined. Problems encountered in applying the method are identified and recommendations to improve the measurement results are provided. These include chamber design, type and placement of transmitting and reference receiving antenna, determination and correction for VSWR of the reference antenna and equipment under test (EUT), and the measurement approach to use at specified test frequencies. Design and measurement setups for a small mode-stirred chamber suitable for performing SE measurements in the frequency range (1-18)GHz with dynamic ranges up to 130 dB are given along with SE measurement results of some sample EUTs.

100,777 PB92-117324 Not available NTIS National Inst. of Standards and Technology (EEEL), Boulder, CO. Electromagnetic Fields Div. Air Gage Size Measurement of Microwave Standards.

Final rept G. V. Sherwood. 1991, 10p

Pub. in Proceedings of Measurement Science Conference, Anaheim, CA., January 31-February 1, 1991, p1-

Keywords: \*Transmission lines, \*Coaxial cables, \*Waveguides, \*Standards, Dimensional measurement, Microwave equipment, Surface roughness, Mechanical measurement, Metrology, Calibration, Reprints.

Size measurement of wave guides and coaxial transmission line standards has been performed at NIST for many years. Recently, the air gaging systems used to perform these measurements have been enhanced using digital data acquisition methods to facilitate computer analysis. Initial experiments were performed using air gaging probes on a coordinate measuring machine to correlate linear position with size attributes. Related geometric and dimensional characteristics that contribute to the uncertainty of measurement were also studied. Alternative assessment methods have been used to provide a more complete characterization of these features and complement air gage size measurements using a systems approach. The article is a report of these developments at NIST.

### Resistive, Capacitive, & Inductive Components

100,778 **N91-25797/2** 

(Order as N91-25755/0, PC A99/MF A04) National Inst. of Standards and Technology (NML), Boulder, CO. Time and Frequency Div.

Environmental Sensitivities of Quartz Crystal Oscillators. F. L. Walls. May 90, 22p

Pub. in Proceedings of Annual Precise Time and Time Interval (PTTI) Applications and Planning Meeting (22nd) p465-486 (See N91-25755 17-70).

Keywords: \*Crystal oscillators, Frequencies, Quartz crystals, Sensitivity, Electric fields, Humidity, Loads (Forces), Magnetic fields, Precision, Pressure distribution, Vibration, \*Quartz resonators.

The frequency, amplitude, and noise of the output signal of a quartz crystal controlled oscillator is affected by a large number of environmental effects. The physical basis for the sensitivity of precision oscillators to temperature, humidity, pressure, vibration, magnetic field, electric field, load, and radiation is discussed. The sensitivity of crystal oscillators to radiation is a very complex topic and poorly understood. Therefore only a few general results are mentioned. The sensitivity to most external influences often varies significantly from one oscillator type to another and from one unit of given type to another. For a given unit, the sensitivity to one parameter often depends on the value of other parameters and history.

100,779 PB91-134320 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Temperature and Pressure Div. Stability of Thermistors.

Final rept.

B. W. Mangum. 1987, 6p

Pub. in Proceedings of International Symposium on Temperature Measurement in Industry and Science, p170-175 1987.

Keywords: \*Thermistors, \*Thermal stability, Aging tests(Materials), Reprints.

Thirty-two bead-in-glass probe-type and 67 disc-type thermistors from six manufacturers have been investigated for stability upon thermal cycling from 0 to 300 or 150C for the beads and 0 to 100C for the discs. Also, 12 bead-in-glass probes and 11 discs were aged for about 4000 hours at 100C. After the thermistors were heat treated at the elevated temperatures, their resistances were measured over the range from 0 to 100C. The disc-type thermistors were much less stable than the bead-in-glass probe types. The bead thermistors were not very stable when subjected to 300C environ-ments nor were the discs when subjected to 100C environments.

PB91-134338 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Temperature and Pressure Div. SRM 1970 - Succinonitrile Triple-Point Standard -

And Its Use in Calibration of Thermistors.

Final rept. B. W. Mangum. 1987, 6p

Pub. in Proceedings of International Symposium on Temperature Measurement in Industry and Science,

Keywords: \*Thermistors, Reprints, \*Standard reference materials, \*Succinonitrile, \*Calibration.

The triple-point temperature of succinonitrile (SCN) has been found to be a good reference point at about

58.08 C, a value in a region devoid of fixed points. Cells with reentrant wells and containing approximately 60 grams of zone-refined SCN have been investigated for use as a Standard Reference Material (SRM), SRM 1970. They were designed to accept thermistor thermometers primarily, but will accept any thermometer that is less than 4.5 mm in diameter. Through a three-point calibration obtained by the use of SRM 1970, SRM 1968 (the Gallium Melting-Point Standard), and the triple point of water, thermistors can be calibrated with an uncertainty as small as + or - 2 or 3 mK over the range from 0 to 70 C.

100.781 PB91-134866 Not available NTIS National Bureau of Standards (NML), Boulder, CO. Time and Frequency Div.

Environmental Effects on the Medium and Long Term Frequency Stability of Quartz Oscillators. Final rept.

F. L. Walls. 1988, 9p

Pub. in Proceedings of European Frequency and Time Forum (2nd), Neuchatel, Switzerland, March 16-18, 1988, p719-727.

Keywords: \*Quartz resonators, \*Frequency stability, Environmental tests, Atomic clocks, Pressure, Humidity, Frequency standards, Reprints.

The medium and longterm frequency stability of most quartz oscillators is degraded by various environmental effects, the most important of which appear to be acceleration, temperature, load change, pressure, and possibly humidity. In the paper, preliminary data are shown which indicate that the medium and long term frequency stability of some ocillators can be improved by controlling the pressure and humidity around the oscillator. These data were obtained on only one oscillator of each type and may or may not be representative. If these improvements can be obtained in other precision crystal oscillators, then crystal oscillators may become usable in some applications generally thought to require atomic standards.

100.782 PB91-174912 Not available NTIS National Inst. of Standards and Technology (NEL), Boulder, CO. Electromagnetic Technology Div.
Noise-Affected I-V Curves in Small Hysteretic Josephson Junctions. Final rept.

R. L. Kautz, and J. M. Martinis. 1990, 35p Sponsored by Office of Naval Research, Arlington, VA. Pub. in Physical Review B 42, n16 p9903-9937, 1 Dec

Keywords: \*Josephson junctions, Electromagnetic noise, Quasi particles, Hysteresis, Reprints.

The authors investigate the noise-affected I-V curves of small-area Josephson junctions through experiment, simulation, and theory. In particular, the authors consider I-V curves in which two different states of finite voltage coexist at the same de bias: a high-voltage state that corresponds to the usual quasiparticle branch and a low-voltage state that is characterized by thermally activated phase diffusion. In addition, the authors develop analytic expressions for three key parameters of the I-V curve of junctions displaying hysteresis between the phase-diffusion and quasiparticle branches: the initial slope of the phase-diffusion branch, the bias level at which the junction switches from the phase-diffusion branch to the quasiparticle branch, and the bias level at which it returns to the phase-diffusion branch.

100,783 PB91-190116 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Chemical Process Metrology Div. Transparent Thin Film Thermocouple. Final rept. M. Yust, and K. G. Kreider. 1989, 6p See also PB91-110635. Pub. in Thin Solid Films 176, n1 p73-78 Sep 89.

Keywords: \*Thin films, \*Thermocouples, \*Indium oxides, \*Tin oxides, Sputtering, Ceramics, Transparence, Platinum, Calibrating, Temperature measuring instruments, Reprints.

A transparent thin film thermocouple has been produced by reactive sputtering which has a Seebeck co-efficient of 0.14 mv/C. The positive leg of the thermocouple is indium tin oxide (ITO) and the negative leg is

### Resistive, Capacitive, & Inductive Components

indium oxide (In203). The In203 and ITO thin films were also tested with sputtered thin film platinum to obtain their individual thermoelectric potentials. Stability of the transparent thermocouple at 575K and calibration data of sputtered ITO and platinum are also reported.

100 784

PB91-195446 Not available NTIS National Inst. of Standards and Technology (NEL), Boulder, CO. Electromagnetic Technology Div. Sidelobe Suppression in Small Josephson Junc-

tions. Final rept. R. L. Peterson. 1991, 4p Pub. in Cryogenics 31, p132-135 Feb 91.

Keywords: \*Josephson junctions, \*Critical current, Diffraction patterns, Sidelobes, Reprints.

Many applications of Josephson junctions require that the sidelobes of the critical-current patterns as a function of magnetic field be as small as possible. The sidelobes can be significantly suppressed by appropriate choice of junction geometry. The paper emphasizes that suppression is not just a long-junction effect. For a wide variety of shaped small junctions, the diffraction patterns are given by simple expressions, in-spection of which quickly shows the overall features of the patterns. For some shapes the highest sidelobes can be kept well under 1% of the central lobe. For applications requiring long junctions, the geometry of small junctions giving the desired pattern is a practical

starting point for a long-junction analysis.

### Semiconductor Devices

100.785 DE91002169 PC A03/MF A01 Solar Energy Research Inst., Golden, CO. Scanning tunneling microscopy studies of the surfaces of a-Si:H and a-SiGe:H films. Annual report, 1 December 1989-31 January 1991.

Progress rept.
A. Gallagher, R. Ostrom, and D. Tannenbaum. Jun
91, 35p SERI/TP-214-4409
Contract AC02-83CH10093

Sponsored by Department of Energy, Washington, DC.

Keywords: \*Germanium Compounds, \*Silicon Compounds, Amorphous State, Chemical Reactions, Chemical Vapor Deposition, Electric Discharges, Etching, Hydrogen Compounds, Microstructure, Progress Report, Scanning Electron Microscopy, Silanes, Solar Cells, Stoichiometry, Thin Films, EDB/360602, EDB/140501, EDB/400102.

The report contains a detailed description of the experimental complexities encountered in developing scan-ning tunneling microscope (STM) probing of atomic structure on the surface of freshly-grown hydrogenat-ed-amorphous semiconductors. It also contains a speculative microscopic film-growth model that ex-plains differences between the disorder in CVD grown a-Ge:H versus a-Si:H films. This model is derived from prior results obtained in the chemical analysis of GeH(sub 4) plasmas, combined with surface reaction and thermodynamic considerations. The neutral radical fragments of silane, disilane and germane dissocia-tion in discharges, which dominate the vapor and film-growth reactions, have been deduced from detailed analysis of prior data and are reported. 4 refs., 7 figs.

100,786 PB91-134692 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Semiconductor Electronics Div.
Current Density Dependence of Electromigration
t50 Enhancement Due to Pulsed Operation.

Plila rept.

J. S. Suehle, and H. A. Schafft. 1990, 5p

Pub. in Proceedings of Annual Conference on Reliability Physics 1990 (28th), New Orleans, LA., March 27-29, 1990, p106-110.

Keywords: \*Integrated circuits, Reliability(Electronics), Current density, Metallizing, Reprints, \*Electromigration, Electric pulses.

Two effects that complicate the electromigration characterization of metallization for pulsed stress have been observed. One is the dependence of the t(50) enhancement (due to pulsed operation) on current density and the other is a decrease of this enhancement over a range of frequencies (0.2 to 2 MHz) that is connected with the joule heating. These effects are discussed in terms of changes in the buildup and relaxation response times of the excess vacancy concen-

100.787

PB91-147181 Not available NTIS National Inst. of Standards and Technology (NEL), Boulder, CO. Electromagnetic Technology Div.
Low-Temperature, Electrically Calibrated SOS Bolometer for Power and Energy Measurements.

R. M. Craig, and R. J. Phelan. 1990, 11p Sponsored by Aerospace Guidance and Metrology Center, Newark AFS, OH.

Pub. in Proceedings of Measurement Science Conference, Anaheim, CA., February 8-9, 1990, p3A-1-3A-11

Keywords: \*Bolometers, Visible radiation, Infrared radiation, Power measurement, Radiometry, Cryogenics, Reprints, SOS(Semiconductors), Silicon on sapphire.

A system has been constructed to allow absolute, electrically calibrated radiometry of low power (pW/Hz to the 1/2 power) and low energy (pJ) beams. The detector is based on an adaptation of silicon-on-sapphire (SOS) technology with an integral absorber/heater for real-time electrical substitution. Cooling is provided by a custom closed-cycle helium liquefaction system built inside an optical access Dewar. Convenient control and data analysis are provided by use of the GPIB bus and a computer. This arrangement will allow routine laser measurements and detector calibrations at 1%-5% accuracy across the 0.4 micrometer to 15 micrometers wavelength range.

PB91-147520 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Semiconductor Electronics Div. Verification of the Relation between Two-Probe and Four-Probe Resistances as Measured on Silicon Wafers. Final rept.

J. J. Kopanski, J. Albers, G. P. Carver, and J. R.

Ehrstein. 1990, 7p Pub. in Jnl. of the Electrochemical Society 137, n12 p3935-3941 Dec 90.

Keywords: \*Electrical resistance, \*Silicon, Electrical measurement, Probes(Electromagnetic), Laplace equation, Wafers, Reprints, Spreading resistance, Mul-

The predicted relation between the two-probe resistance (spreading resistance) and the four-probe resistance, and the dependence of the four-probe resistance on the ratio of layer thickness to probe spacing have been experimentally verified. The verified behavior is predicted from calculations, based upon the soluior is predicted from calculations, based upon the solu-tion of Laplace's equation, of the two- and four-probe resistance for arbitrary, vertical resistivity profiles. Arrays of lithographically fabricated, geometrically well-defined contacts on silicon wafers were utilized to make the necessary precise, reproducible resistance measurements. Additional measurements using point pressure contacts were also made. The dependence of the four-probe resistance on the ratio of layer thick-ness to probe spacing was verified for both the in-line ness to probe spacing was verified for both the in-line and square probe configurations.

100.789

PB91-147819 Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Semiconductor Electronics Div.

Thermal Characterization of Integrated Circuits - A Tutorial.

Final rept

Pub. in Proceedings of Symposium SEMI-THERM 3, Scottsdale, AZ., December 10, 1986, 4p.

Keywords: \*Integrated circuits, Thermal analysis, Computation, Experimentation, Reprints.

The tutorial deals with the practicalities of the thermal characterization of integration of integrated circuit devices and packages, using both computational and experimental techniques.

100,790

PB91-147827 Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Semiconductor Electronics Div.
Thermal Measurements of VLSI Packages: A Criti-

cal Review.

Final rept.

Pub. in Program and Extended Abstracts VLSI Packaging Workshop, Gaithersburg, MD., September 9-11, 1985, p26-29.

Keywords: \*Very large scale integration, \*Integrated circuits, \*Thermal measurements, Computerized simulation, Chips(Electronics), Reviews, Reprints.

Techniques to thermally characterize ceramic and plastic VLSI packages are discussed. Computer simulations and both direct and indirect thermal evaluation techniques are highlighted. Limitations and strengths of the various techniques are identified.

100,791 PB91-147918 Not available NTIS Not available 19113
National Bureau of Standards (NEL), Gaithersburg,
MD. Semiconductor Electronics Div.
Investigation of Photoconductive Picosecond Microstripline Switches on Self-Implanted Silicon on

Sapphire (SOS).

Final rept.
P. Pollack-Dingels, G. Burdge, C. H. Lee, A. C. Seabaugh, R. T. Brundage, M. I. Bell, and J. Albers.

1987, 5p See also PB90-218124.

Pub. in Proceedings of OSA-IEEE (LEOS) Meeting (2nd) Picosecond Electronics and Optoelectronics II, Incline Village, NV., January 14-16, 1987, p232-236.

Keywords: \*Semiconductor switches, Amorphous silicon, Electrical resistivity, Microstrip devices, Ion implantation, Silicon ions, Raman effect, Pholoconductivity, Radiation damage, Lifetime, Reprints, SOS(Semiconductors), Picosecond pulses.

Silicon on sapphire (SOS) switches, damaged by Si implantation at fluence levels of 10 to the 13 power to 10 to the 15 power/sq cm, were characterized by picosecond cross-correlation, Raman, and resistivity measurements.

100 792

PB91-148197 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Semiconductor Electronics Div. Comparison of High-Resistivity Measurements of Silicon by AC Impedance, DC Resistance, van der Pauw, and Four-Probe Methods.

Final rept. W. R. Thurber, J. R. Ehrstein, and J. R. Lowney.

1990, 2p Pub. in Extended Abstracts, Electrochemical Society 1990 Fall Meeting, Seattle, WA., October 14-19, 1990,

Keywords: \*Electrical resistivity, \*Silicon, Electrical impedance, Electrical measurement, pedance, Electrical measurement, Probes(Electromagnetic), Comparison, Reprints.

Resistivity measurements by different techniques are compared for high-resistivity silicon. The ac impedance method is emphasized as it is seldom used for silicon but has certain advantages for high-resistivity material. Slices with implanted and annealed surfaces were measured by the impedance method and twoterminal dc resistance. For material with lapped surfaces, results were obtained by ac impedance, van der Pauw, and four-probe methods. The agreement was within 5% for slices and ingot sections greater than 0.1 cm in length and resistivity above 5 K(ohm)-cm.

100,793 PB91-149062 Not available NTIS National Bureau of Standards (NEL), Gaithersburg,

MD. Semiconductor Electronics Div.
Characteristics of the Breakdown Voltage of Power MOSFETs After Total Dose Irradiation.

R. D. Pugh, A. H. Johnston, and K. F. Galloway.

1986, 5p Sponsored by Air Force Inst. of Tech., Wright-Patter-

son AFB, OH.
Pub. in IEEE (Institute of Electrical and Electronics Engineers) Transactions on Nuclear Science NS-33, n6 p1460-1464 Dec 86.

# Semiconductor Devices

Keywords: \*Field effect transistors, \*MOSFET, \*Radiation effects, \*Breakdown(Electronic threshold), Gamma irradiation, Radiation hardening, Silicon, Re-

The effects of total dose irradiation on the breakdown voltage of p-channel power MOSFETs are examined. Although breakdown voltage for p-channel devices increased at higher dose levels, as expected, some devices exhibited an initial decrease in breakdown at very low levels of total dose. The interaction of ionizing radiation effects with the junction termination methods designed to increase the voltage at which breakdown occurs is analyzed.

100,794 PB91-149070 Not available NTIS National Inst. of Standards and Technology (NEL), Boulder, CO. Electromagnetic Fields Div. MMIC Related Metrology at the National Institute of Standards and Technology. Final rept.

G. R. Reeve, R. Marks, and D. L. Blackburn. 1990,

4p Pub. in Proceedings of IEEE (Institute of Electrical and Electronics Engineers) Instrumentation and Measurement Technology Conference, San Jose, CA., February 13-15, 1990, p196-199.

Keywords: \*Integrated circuits, \*Metrology, Gallium arsenides, Probes(Electromagnetic), Wafers, Reprints, \*MMIC, US NIST.

Last year a program was instituted at the National Institute of Standards and Technology (NIST) specifically directed at developing improved metrology methods and standards to support microwave monolithic integrated circuit (MMIC) technology. The paper describes how the program was developed, the modes of interaction with the industrial community and the DARPA MIMIC initiative, and the particular projects being undertaken which will result in a more consistent measurement base for those engaged in the design and manufacture of MMIC devices.

100,795 PB91-149120 Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Semiconductor Electronics Div. Measurement of Capacitance on Wafers. Final rept.

Pinal rept.
P. Roitman, J. S. Suehle, T. J. Russell, and M. Gaitan. 1986, 9p
Pub. in Proceedings of IEEE (Institute of Electrical and Electronics Engineers) VLSI (Very Large Scale Integration) Workshop on Test Structures, Long Beach, CA., February 17-18, 1986, p96-104.

Keywords: \*Very large scale integration, \*Integrated circuits, \*Capacitance, Electrical measurement, Probes(Electromagnetic), Wafers, Reprints.

Capacitance measurements of both capacitor and transistor structures can provide critical parameters for process monitoring, process modeling, device modeling and circuit modeling. However, accurate measurements of capacitance on small devices located on large silicon wafers are very difficult. The problem is simply that very low level analog measurements must be made at the end of a necessary system of cables and probes. Several authors have proposed building capacitance meters on the wafer, which would provide relatively high level outputs to the external test system. The authors have chosen to improve their capability to measure capacitance on wafers directly. This improvement involved three parts of the experiment: the design of the capacitors, the design of the probe fixturing, and the instrumentation. These are discussed in

100,796 PB91-149880 Not available NTIS Not available NTS
National Inst. of Standards and Technology (NEL),
Gaithersburg, MD. Precision Engineering Div.
Selective-Area Epitaxial Growth of Gallium Arsenide on Silicon Substrates Patterned Using a Scanning Tunneling Microscope Operating in Air. Final rept.

J. A. Dagata, W. Tseng, J. Bennett, C. J. Evans, J. Schneir, and H. H. Harary. 1990, 3p See also AD-A209 079.

Pub. in Applied Physics Letters 57, n23 p2437-2439, 3

Keywords: \*Gallium arsenides, \*Epitaxial growth, Scanning tunneling microscopy, Substrates, Silicon, Reprints, Nanotechnology.

Selective-area epitaxial growth of gallium arsenide on n-Si(100) substrates is reported, where the oxide (SiOx) mask consists of 1-2 monolayer-thick features patterned onto a silicon substrate using a scanning tunneling microscope (STM) operating in air. The technique for generating the STM patterns on hydrogenpassivated silicon was reported recently (1990). The GaAs epilayer was grown by migration-enhanced epitaxy at 580C and its morphology was investigated by scanning electron microscopy. The chemical selectivity of the STM-patterned regions was verified by imaging time-of-flight secondary-ion mass spectrometry. The implications of these results for the development of a unique, STM-based nanostructure fabrication technology are discussed.

100,797 PB91-149989 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Applied and Computational Mathematics Div.

Modelling Gallium Arsenide Transistors. Final rept.

J. L. Blue, and C. L. Wilson. 1990, 9p Pub. in Lectures in Applied Mathematics 25, p89-97

Keywords: \*Transistors, \*Gallium arsenides, \*Mathematical models, Partial differential equations, Monte Carlo method, Quantum mechanics, Thermodynamics,

The usual equations used in modelling semiconductor devices are a set of three coupled partial differential equations first formulated forty years ago. These PDEs are adequate to model present-day silicon transistors, but are inadequate for modelling GaAs transistors. Suitable PDEs can be formulated using quantum mechanics and statistical thermodynamics models obtained by Monte-Carlo calculations.

100,798 PB91-158873 Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Precision Engineering Div.

NBS Submicron Particle Standards for Microcontamination Measurement.

Final rept

T. R. Lettieri. 1989, 7p

Pub. in Semiconductor Fabrication: Technology and Metrology, ASTM STP 990, p215-221 1989.

Keywords: \*Semiconductor devices, \*Standards, Contamination, Microspheres, Substrates, Silicon, Surfaces, Wafers, Reprints, \*Particle standards, US NIST.

There is a recognized need for standard artifacts with which to calibrate the laser-scanning instruments which detect and monitor microcontamination on semiconductor wafers. Although commercial calibration wafers are available for this purpose, the present paper proposes the use of National Bureau of Standards (NBS) particle-sizing standard microspheres, de-posited on polished silicon substrates, as an alterna-tive working standard until such time as a true national calibration artifact is developed. To this end, several techniques for depositing the microspheres on semi-conductor surfaces are presented in the paper. In addition, the technques used to certify the NBS particle standards and the measurement results from each technique are summarized.

PB91-159087 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Precision Engineering Div. Submicrometer SEM Magnification Standard.

M. T. Postek, and R. C. Tiberio. 1989, 4p Pub. in National Nanofabrication Facility Research Accomplishments 1988-89, 4p 1989.

Keywords: \*Dimensional measurements, \*Scanning rephy, Prototypes, Reprints, \*Magnification standards, Nanofabrication, Standard reference materials.

The National Institute of Standards and Technology (NIST) in conjunction with the National Nanofabrication Facility (NNF) has had a continuing effort for the development of a submicrometer scanning electron microscope (SEM) magnification standard prototype. The program is one portion of a feature-size measure-ment program specifically aimed at the development and certification of SEM magnification and linewidth standards and the associated techniques for their calibration and use. The program has several distinct tasks that have undergone simultaneous development at NIST (Postek et al., 1987, Postek et al., 1989, Postek, 1989). One of these tasks has been the development and fabrication of a lithographically produced submicrometer SEM magnification standard useful at low accelerating voltages. With the assistance of the NNF, a prototype magnification standard has been fabricated and has undergone further refinements in materials selection and etching techniques during the

100.800

Not available NTIS PB91-159244 National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Semiconductor Electronics Div. Permittivity Measurements on Molecular-Sized Samples. Final rept.

A. van Roggen, L. Yuwono, H. Zhou, P. H. E. Meijer, and J. J. Kopanski. 1990, 6p

Sponsored by National Science Foundation, Washing-

Pub. in Proceedings of Conference on Electrical Insulation and Dielectric Phenomena, Pocono Manor, PA., October 29-31, 1990, p385-390.

Keywords: \*Molecular electronics, \*Organic semiconductors, \*Permittivity, Measurement, Polyethylene, Reprints.

A new laboratory on Molecular Electronics has been started at the Physics Department of the Catholic University of America. In their efforts to make organic bistable devices, one of the research functions of the laboratory is to measure the electrical properties of materials and active devices made with molecular (mainly organic) materials. The size of material samples, and the specimens used for measurement, is exceedingly small, typically layers with a thickness of the order of 100 nm. Consequently, the setups used for normal dielectric and conductivity measurements = or > 10 mm electrode size) cannot be used, and special cells and instrumentation have to be developed.

100.801 PB91-159749 PC A03/MF A01 National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Semiconductor Electronics Div. Center for Electronics and Electrical Engineering Technical Progress Bulletin Covering Center Programs, July to September 1990, with 1991 CEEE Events Calendar. J. A. Gonzalez. Jan 91, 48p NISTIR-4496 See also PB91-107201.

Keywords: \*Semiconductor devices, \*Metrology, Electromagnetic interference, Optical fibers, Integrated circuits, Antennas, Silicon, Electrooptics, Superconductors, Signal processing, Waveforms, Progress report, US NISŤ

The report is the thirty-second issue of a quarterly publication providing information on the technical work of the National Institute of Standards and Technology (formerly the National Bureau of Standards) Center for (formerly the National Bureau of Standards) Center for Electronics and Electrical Engineering. The issue of the CEEE Technical Progress Bulletin covers the third quarter of calendar year 1990. Abstracts are provided by technical area for both published papers and papers approved by NIST for publication. General topics discussed include the following: Semiconductor Technology Program; Signals and Systems Metrology Program; Additional Information; 1991 CEEE Calendar: Sponsor List and Key Contacts in Center. Center dar; Sponsor List; and Key Contacts in Center, Center Organization.

100.802 PC A03/MF A01 PB91-167163 National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Center for Mfg. Engineering. Standard Reference Materials: Bright-Chromium Linewidth Standard, SRM 476, for Calibration of Optical Microscope Linewidth Measuring Systems.

Special pub (Final). C. F. Vezzetti, R. N. Varner, and J. E. Potzick. Jan 91, 47p NIST/SP-260/114

Also available from Supt. of Docs. as SN003-003-03047-3.

Keywords: \*Integrated circuits, \*Dimensional measurement, \*Optical microscopes, \*Calibration, \*Photomasking, \*Line width, Process control, Precision, Chromium, \*Standard reference materials.

### Semiconductor Devices

Standard Reference Material, SRM 476, was developed for use in calibrating optical microscopes used to measure linewidths in the range of 0.9 to 10.8 micrometers on bright chromium photomasks, such as those used in the production of integrated circuits. The SRM, the measurement system, and the procedures used to calibrate the SRM are described. The algorithm for determining the line edge location uses a threshold crite-rion derived from analysis of microscope image profiles. The profiles are predicted by computer modeling based on the theory of partial coherence. The performance of the system is monitored by measuring line features on a control photomask before and after calibrating each SRM. Precautions concerning care and handling and instruction for the use of SRM 476 to calibrate optical microscopes for photomask linewidth measurement are given.

Not available NTIS Not available NTIS
National Bureau of Standards (NEL), Gaithersburg,
MD. Semiconductor Devices and Circuits Div.
Design, Fabrication, and Testing of an Interconnect Test Structure for Evaluating VLSI Processes.

Final rept.

M. W. Cresswell, E. S. Coleman, W. D. Partlow, and

L. W. Linholm. 1985, 2p Pub. in Proceedings of Government Microcircuit Appli-cations Conference, Orlando, FL., November 5-7, 1985, p359-360.

Keywords: \*Very large scale integration, \*Integrated circuits, Test equipment, Test methods, Lithography, Fabrication, Aluminum, Silicon, Design, Reprints

The paper describes a systematic approach to the comparative experimental evaluation of alternative sub-micron lithographic methods using microelectronic test structures. Measurements are presented for both polysilicon and aluminum lines with design geometries of 0.6 to 4.0 micrometers. These structures provide unambiguous results which can be used as a tool to improve the control and performance of VLSI devices.

100,804 PB91-175000 Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Semiconductor Devices and Circuits Div. Characterizing VLSI Processes Using Test Struc-

L. W. Linholm, J. A. Mazer, and K. F. Galloway.

Final rept

1985, 3p Pub. in Proceedings of Digest of the DOD/NBS Conference on Microelectronic Electromagnetic Susceptibility, Gaithersburg, MD., March 12-13, 1985, p16-18.

Keywords: \*Very large scale integration, \*Integrated circuits, Test equipment, Test methods, Electromagnetic interference, Microelectronics, Wafers, Reprints.

Functional tests alone cannot fully evaluate complex integrated circuits (ICs). Comprehensive test programs are needed to assure, with acceptable confidence, that desired performance has been built into these circuits. Results from measurements obtained using specially designed microelectronic test structures can be an important element in a comprehensive test program to assure circuit performance and reliability. In the paper, six categories of test structures are identified and the step at which they impact VLSI circuit production is indicated. An example of the use of test structures is given. Finally, a brief discussion considering the use of test structures for measurements important to understanding effects such as electromagnetic interference (EMI) is given.

100,805 PB91-175489 National Bureau of Standards (NEL), Gaithersburg, MD. Semiconductor Electronics Div.

Evaluation and Improvement of E-Beam Exposure Routines by Use of Microelectronic Test Structures. Final rept.

T. W. O'Keeffe, M. W. Cresswell, L. W. Linholm, and D. J. Radack. 1986, 13p Pub. in Proceedings of IEEE VLSI Workshop on Test Structures, Long Beach, CA., February 17-18, 1986,

p82-94.

Keywords: \*Very large scale integration, \*Integrated circuits, Test equipment, Test methods, circuits, Test equipment, Test methods, Chips(Electronics), Electron beams, Microelectronics, Line width, Reprints.

The paper describes the use of the cross-bridge test structure in conjunction with a series of interconnect test structures to assess and improve the exposure routines and procedures in the replication of submicron features. The interconnect test structures used in the experiment are resistors which include both serpentine and comb-like interconnect patterns and can be used to assess line continuity and line-to-line isolation. Results obtained during the evaluation of line continuity, resolution, linewidth, and proximity exposure effects are presented.

100,806 PB91-189399 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Semiconductor Electronics Div. Uniform Junction Temperature AlGaAs/GaAs Power Heterojunction Bipolar Transistors on Silicon Substrates.

G. Gao, Z. Fan, D. L. Blackburn, M. S. Unlu, J. Chen, K. Adomi, and H. Morkoc. 1991, 3p Sponsored by Air Force Office of Scientific Research, Bolling AFB, DC. Final rept.

Pub. in Applied Physics Letter 58, n10 p1068-1070, 11

Keywords: \*Bipolar transistors, Aluminum gallium arsenides, Thermal stability, Heterojunctions, Substrates, Silicon, Reprints, Power transistors.

AlGaAs/GaAs power heterojunction bipolar transistors on Si substrates exhibiting uniform junction temperature distribution are reported. Owing to a unique device design, the temperature spread across the entire device area is about 1 deg C. The device exhibits a common emitter current gain of 20, a maximum collector current of 0.6 A, and a collector base junction breakdown voltage of 25 V.

100.807 PB91-189779 Not available NTIS
National Inst. of Standards and Technology (NML),
Gaithersburg, MD. Inorganic Analytical Research Div.
Neutron Activation Analysis in Electronic Technology ogy. Final rept.

R. M. Lindstrom. 1988, 1p Pub. in Jnl. of the Electrochemical Society 135, n8 pC372 1988

Keywords: \*Neutron activation analysis, Chemical analysis, Trace amounts, Semiconductors, Silicon, Reprints.

The procedure of neutron activation analysis is reviewed, with recent examples of the application of this and other nuclear analytical methods in semiconductor technology. These methods in many situations offer highly specific and sensitive elemental analysis capability, often wholly instrumental. The sample physics involved in neutron activation in many cases make systematic errors different in kind and less important in quantity than in analytical methods relying on atomic phenomena.

100,808 PB91-194712 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Precision Engineering Div. Pattern Generation on Semiconductor Surfaces by a Scanning Tunneling Microscope Operating in Air.

J. A. Dagata, J. Schneir, H. H. Harary, J. Bennett, and W. Tseng. 1991, 5p Pub. in Jnl. of Vacuum Science and Technology B 9, n2 p1384-1388 Mar/Apr 91.

Keywords: \*Semiconductor devices, \*Pattern making, \*Scanning tunneling microscopy, Gallium arsenides, Silicon, Epitaxy, Masking, Surfaces, Scanning electron microscopy, Reprints, Nanotechnology.

Recent results employing scanning tunneling micro-scope-based techniques for the generation of nano-meter-scale patterns on passivated semiconductor surfaces are presented. Preparation and characterization of hydrogen-passivated silicon and sulfur-passivated gallium arsenide surfaces are described, and the determination of the chemical and morphological propdetermination of the chemical and morphological properties of the patterned regions by scanning electron microscopy and time-of-flight secondary ion mass spectrometry are discussed. The authors' demonstration that ultrashallow, oxide features written by scanning tunneling microscope (STM) can serve as an effective mask for selective-area GaAs heteroepitaxy on

silicon is used to illustrate key requirements necessary for the realization of a unique, STM-based nanotechnology.

100.809

Not available NTIS PB91-194829 National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Semiconductor Electronics High Spatial Resolution Mapping of Semiconductor Resistivity. Final rept.

J. J. Kopanski, G. P. Carver, J. R. Lowney, D. S. Miles, and D. B. Novotny. 1991, 2p Pub. in Extended Abstracts, v91-1 p698-699 1991.

Keywords: \*Mercury cadmium tellurides, \*Gallium arsenides, \*Silicon, \*Electrical resistivity, High resolution, Laplace equation, Semiconductors, Lithography, Reprints, \*Resistivity mapping, Spreading resistance.

A new approach to the resistivity mapping of semiconductors uses an array of lithographically defined contacts (at a density of 60,000 sites per sq cm and an automated probe station for data acquisition. Resistivity growth striations in silicon as narrow as 45 micrometers in width and with + or - 5% variation from the background resistivity have been resolved. Solution of the Laplace equation for the measurement geometry and measurements on ion implanted test structures are described. Anticipated applications include resistivity mapping of liquid encapsulated Czochralski GaAs, Hg(1-x)Cd(x)Te, and fine scale resistivity variations in processed silicon.

PB91-203141 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Semiconductor Electronics Div.

Final rept. G. G. Harman. 1989, 13p Pub. in Reliability and Yield Problems of Wire Bonding in Microelectronics, Chapter 5, p141-163 1989.

Keywords: \*Electric contacts, \*Microelectronics, Integrated circuits, Reliability(Electronics), Fracture mechanics, Gallium arsenides, Test methods, Silicon, Failure, Reprints, \*Wire bonds.

The monograph describes the several methods of testing the quality of wire bonds, including the pull test, the shear test, and the high-temperature stress test. Essentially all metallurgical, chemical, and mechanical bond failure modes are described, including cratering, 'plaque,' the effect of various contaminants, cleaning and cleaning methods, poor bonding machine control, and the effect of external environments. Methods of preventing or detecting these failures are given. In conclusion, how 'new technology' processing and packaging have changed classical wire bond failures is discussed. Discussion of proposed 'new' wire and pad metallizations and general guidelines for anticipating the reliability of such new materials is also given.

100,811 PB91-203752 Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Precision Engineering Div.

New Approach to Image Modeling and Edge Detection in the SEM.

Final rept.

r-inal rept.

D. Nyyssonen. 1988, 9p
Sponsored by CD Metrology, Inc., Germantown, MD.
Pub. in Proceedings of SPIE (Society of Photo-Optical Instrumentation Engineers) - Integrated Circuit Metrology, Inspection, and Process Control II, v921 p48-56 1988.

Keywords: \*Scanning electron microscopy, \*Edge detection, \*Imaging techniques, \*Very large scale integration, Probability density functions, Monte Carlo method, Electron scattering, Integrated circuits, Process control, Line width, Reprints, Secondary electrons, Micrometrology.

The need for feature-size measurements on microchips for VLSI and other developing technologies with micrometer and submicrometer dimensions has resulted in the use of scanning electron microscopes (SEMs) for process control measurements. However, good measurement practice requires the ability to accurately predict the observed signal output for any given structure of the feature. The model forms the basis for measurement algorithms, error analysis, and proper calibration techniques. The SEM, especially for

### Semiconductor Devices

secondary electron imaging and low beam voltages, has lacked the ability to quantitatively predict image structure at the 0.01 micrometer level needed for submicrometer dimensional control. A new approach to secondary-electron image modeling has been developed consisting of a surface integral (over the line structure) of a probability density function which describes the likelihood of a secondary electron being generated by the primary beam and emitted at a given point in space, if that point coincides with the surface of a line structure. This probability density function can be determined by using either a state-of-the-art Monte Carlo technique or by using a modified diffusion model. The calculation of the image from this probability density function takes into account edge geometry and shadowing due to nearby edges as well as field effects due to any bias voltage on the electron-detector grid.

100,812 PB91-203992 PB91-203992 Not available NTIS
National Inst. of Standards and Technology (NEL),
Gaithersburg, MD. Semiconductor Electronics Div.
Building-in Reliability: Making It Work.
Final rent

H. A. Schafft, D. A. Baglee, and P. E. Kennedy.

1991, 7p Contract ARPA-3882

Sponsored by Defense Advanced Research Projects

Agency, Arlington, VA. Pub. in Proceedings of International Reliability Physics Symposium, Las Vegas, NV., April 9-11, 1991, p1-7.

Keywords: \*Reliability(Electronics), Microelectronics, Semiconductor devices, Process control, Quality control, Packaging, Measurement, Reprints.

Aggressive reliability and market-entry demands will require the use of a building-in approach to reliability. To adopt this approach and make it work requires that very significant breaks be made from the traditional ways of improving and appraising reliability. The nature of these breaks are discussed in the context of describing the basic elements of the approach of building-in reliability and the obstacles that hinder its adop-tion. To help visualize how the approach can be imple-mented, initial steps to make the transition and some specific examples of its use are described.

100,813 PB91-216739

(Order as PB91-216705, PC A07/MF A01) National Inst. of Standards and Technology, Gaithers-

burg, MD.
Automated Reverse-Bias Second-Breakdown

Transistor Tester.
D. Berning. 1991, 14p
Included in Jnl. of Research of the National Institute of Standards and Technology, v96 n3 p291-304 May/Jun

Keywords: \*Nondestructive tests, \*Transistors, \*Second breakdown, Power transistors, Reverse bias.

An automated instrument is described for generating curves for the reverse-bias, safe-operating area of transistors nondestructively. A new technique for detecting second breakdown that makes automation possible is highlighted. Methods to reduce stress to the device under test are discussed, as are several other innovations that enhance automation. Measurements using the tester are described, and limitations on nondestructive testability are discussed.

100,814 PB91-236513 Not available NTIS Not available NTIS
National Inst. of Standards and Technology (EEEL),
Gaithersburg, MD. Semiconductor Electronics Div.
Automated Reverse-Bias Second-Breakdown
Transistor Tester. Final rept.

D. W. Berning. 1991, 8p
Pub. in Proceedings of Applied Power Electronics Conference and Exposition, Dallas, TX., March 10-15, 1991, p339-346.

Keywords: \*Transistors, Electromagnetic testing, Non-destructive tests, Automation, Reprints, \*Second breakdown, Reverse bias.

An automated instrument is described for generating curves for the reverse-bias, safe-operating area of transistors nondestructively. A new technique for detecting second breakdown that makes automation possible is highlighted. Methods to reduce stress to the device under test are discussed, as are several other innovations that enhance automation. Measure-

ments using the tester are described, and limitations on nondestructive testability are discussed.

PB91-236703 Not available NTIS National Inst. of Standards and Technology (CSL), Gaithersburg, MD. Systems and Software Technology

Emitter Ballasting Resistor Design for, and Current Handling Capability of AlGaAs/GaAs Power Heterojunction Bipolar Transistors.

Final rept. G. Gao, M. S. Unlu, H. Morkoc, and D. L. Blackburn. 1991, 12p

Pub. in IEEE (Institute of Electrical and Electronics Engineers) Transactions on Electron Device 38, n2 p185-196 Feb 91.

Keywords: \*Bipolar transistors, Aluminum gallium arsenides, Thermal analysis, Heterojunctions, Resistors, Reprints, Power transistors, Emitter ballasting.

A systematic investigation of the emitter ballasting resistor for power Heterojunction Bipolar Transistors (HBTs) is presented. The current-handling capability of power HBTs is found to improve with ballasting resistance. An equation for the optimal ballasting resistance is presented, where the effects of thermal conductivity of the substrate material and the temperature coefficient of the ballasting resistor are taken into account. Current levels of 400 to 800 mA/mm of emitter periphery at case temperatures of 25 to -80 C for power AlGaAs/GaAs HBTs have been obtained using an on-chip lightly-doped GaAs emitter ballasting resistor. Device temperature has been measured using both an infrared micro-radiometer and temperature-sensitive electrical parameters. Steady-state and transient thermal modeling were also performed. Although the measured temperature is spatially nonuniform, the modeling results show that such nonuniformities occur for a uniform current distribution, as is to be expected for an HBT with emitter ballasting resistors.

P891-237255 Not available NTIS National Inst. of Standards and Technology (NEL), Boulder, CO. Electromagnetic Fields Div.

Microwave Monolithic Integrated Circuit-Related Metrology at the National Institute of Standards and Technology. Final rept.

G. R. Reeve, R. Marks, and D. L. Blackburn. 1990,

Pub. in IEEE (Institute of Electrical and Electronics Engineers) Transactions on Instrumentation and Measurement 39, n6 p958-961 Dec 90.

Keywords: \*Integrated circuits, \*Metrology, Microwave circuits, Gallium arsenides, Probes(Electromagnetic), Wafers, Reprints, US NIST.

The paper describes how the National Institute of Standards and Technology (NIST) interacts with the GaAs community and the Defense Advanced Research Projects Agency (DARPA) MIMIC initiative. The organization of a joint industry and government labora-tory consortium, for MIMIC related metrology research is described, along with some of the initial technical developments at NIST done in support of the consorti-

100,817 PB91-240739 PC A03/MF A01 National Inst. of Standards and Technology (EEEL), Gaithersburg, MD.

Metrology for the Semiconductor Industry. R. I. Scace. Sep 91, 47p NISTIR-4653

Keywords: \*Integrated circuits, \*Metrology, Semiconductor devices, Semiconductor materials, Microwave equipment, Process control, Optoelectronics, Manufacturing, Automation, Market surveys, \*Semiconductivity, Automatical Semiconductivity, Automatical Semiconductivity, Automatical Semiconductivity, Automatical Semiconductivity, \*Semiconductivity, Automatical Semiconductivity, Automatical Semiconductivity, Automatical Semiconductivity, Automatical Semiconductivity, \*Semiconductivity, Automatical Semiconductivity, \*Semiconductivity, \*Semiconduct tor industry.

The metrological needs of the semiconductor industry and its supporting materials and manufacturing equip-ment industries for the 1990's are set forth. The information in the report derives from technological workshops sponsored by the American Society for Testing and Materials, NIST, SEMATECH, Semiconductor Equipment and Materials International, and the Semiconductor Research Corporation; from industry information sources such as Dataquest and VLSI Re-search; from NIST colleagues; and from personal discussions with many others in the field. The data from these sources have been analyzed for their implications for measurement science and technology, on which the report focuses. It contains a brief introduction to the economic significance of the semiconductor industry, an overview of the relevant technologies, their development trends and the metrological needs thus implied, and evidence of needs expressed by sources outside of NIST. The report deals with the needs for measurements of all kinds, but intentionally does not discuss the means by which these may be met. The text is also to be published as one chapter in a more comprehensive assessment covering the electronics industry as a whole.

100,818

Not available NTIS PB92-116466 National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Scientific Computing Div.

Three-Dimensional Simulations of High-Resolution Photoresist Processing.

Final rept.

E. Barouch, B. Bradie, and H. A. Fowler. 1991, 12p Sponsored by Defense Advanced Research Projects Agency, Arlington, VA., and Air Force Office of Scientific Research, Bolling AFB, DC.

Pub. in Jnl. of Imaging Science 35, n4 p240-251 Jul/

Keywords: \*Integrated circuits, \*Computerized simulation, Computer graphics, Three dimensional, Dissolving, Reprints, \*Microlithography, Photoresists.

A computer simulation package for optical microlithography contains modules for the processing of positive photoresists in the three stages of aerial-image transfer, exposure-bleaching, and dissolution. Evolving and final resist profiles are displayed in three dimensions at several dissolution times, thus simulating real systems in their natural form. Results presented for a variety of examples demonstrate the robustness and versatility of the package.

100,819

Not available NTIS PB92-116599 National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Semiconductor Electronics Div. Ellipsometry SRM's for Use in Thin Film Measurements.

Final rept.

D. Chandler-Horowitz, J. F. Marchiando, and B. J. Belzer. 1990, 11p

Pub. in Proceedings of Measurement Science Conference, Anaheim, CA., February 8-9, 1990, p5A-11-5A-

Keywords: \*Silicon dioxide, \*Film thickness, \*Dimensional measurement, \*Ellipsometry, Helium neon lasers, Refractive index, Thin films, Polarimetry, Semiconductors, Reprints, \*Standard reference materials.

A Standard Reference Material (SRM) consisting of a film of silicon dioxide on a silicon substrate has been designed, fabricated, measured, and certified at NIST for the ellipsometric angles, Delta and psi, and for the derived film thickness and refractive index. The SRM can be used as an aid in the evaluation of the performance of optical and mechanical thickness-monitoring instruments as well as ellipsometers. The optical instruments are based on the theory describing reflec-tion of light from a sample. The film thickness is determined by using a model having one or two uniform isotropic films atop a substrate. The calculated thicknesses rely on accurate values of the indices of refraction of the substrate and/or film at the necessary frequencies of light. The measurement procedure used here to certify the ellipsometric angles uses an accurate rotating-analyzer ellipsometer and HeNe laser source operating near the principal angle of incidence. The measurement data from several samples are analyzed collectively to determine the certified film thicknesses and refractive index. At the present time, three different film thicknesses, 50, 100, and 200 nm, are being certified. Future work may involve certifying thinner layers of oxide.

100,820

PB92-116607 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Semiconductor Electronics Div.

### Semiconductor Devices

Sensitivity of Ellipsometric Modeling to the 'Islands' of Silicon Precipitates at the Bottom of the Buried Oxide Layer in Annealed SIMOX.

Final rept.

D. Chandler-Horowitz, J. F. Marchiando, M. Doss, S. Krause, and S. Visitserngtrakul. 1990, 2p Pub. in Proceedings of IEEE SOS/SOI Technology Conference, Key West, FL., October 2-4, 1990, p73-

Keywords: Transmission electron microscopy, Precipitates, Silicon, Sensitivity, Reprints, \*SIMOX, Spectroscopic ellipsometry, Multilayers.

Spectroscopic ellipsometry is a nondestructive probe which can be highly sensitive to the multilayer struc-ture of materials such as SIMOX (Separation by IM-planted OXygen). Recent TEM micrographs of highflux single-implant SIMOX annealed at 1300 C for 6 hours, show 'islands' of silicon precipitates near the bottom of the buried oxide layer. Spectroscopic ellipsometric measurements were performed on these samples at various implant doses and beam current densities to observe how the measured data fit the data theoretically predicted for various models of SIMOX that lead to the presence of these 'islands'.

PB92-116664 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Semiconductor Electronics Div. Modified Sliding Wire Potentiometer Test Structure for Mapping Nanometer-Level Distances.

M. W. Cresswell, M. Gaitan, R. A. Allen, and L. W.

Linholm. 1991, 6p Pub. in Proceedings of IEEE (Institute for Electrical and Electronics Engineering) International Conference on Microelectronic Test Structures, Kyoto, Japan, March 18-20, 1991, v4 n1 p129-134.

Keywords: \*Potentiometers(Instruments), \*Dimensional measurement, Wafers, Reprints, X ray lithography, Nanometer measurement.

The paper presents a modified voltage-dividing potentiometer test structure which overcomes a problem typical in scaling electrical test structures; it provides a correction for electrical length shortening of a resistor strip caused by the attachment of voltage taps of non-negligible width. The test structure was implemented in chrome on quartz, and measurements of displacements between 10 and 500 nm with + or - 12-nm random error were made using available test equipment. Applications for the test structure may include: monitoring the self-registration accuracy and precision of primary pattern generator systems and monitoring level-to-level overlay in advanced wafer fabrication.

### 100,822

Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Semiconductor Electronics Div. Experimentally Verified IGBT Model Implemented in the Saber Circuit Simulator.

A. R. Hefner, and D. M. Diebolt. 1991, 10p Pub. in Proceedings of Annual IEEE (Institute for Electrical and Electronics Engineers) Power Electronics Specialists Conference (22nd), Cambridge, MA., June 24-27, 1991, p10-19.

Keywords: \*Bipolar transistors, Reprints, \*Circuit simulators, Saber model, Power transistors.

A physics-based IGBT (Insulated Gate Bipolar Transistors) model is implemented into the general purpose circuit simulator Saber (TM). The IGBT model includes all of the physical effects that have been shown to be important for describing IGBTs, and the model is valid frequently that the school of the control of the cont for general external circuit conditions. The Saber IGBT model is evaluated for the range of static and dynamic conditions in which the device is intended to be operated, and the simulations compare well with experimental results for all of the conditions studied.

### 100,823

PB92-116920 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Semiconductor Electronics Div.

Test Chip for the Evaluation of Surface-Diffusion Phenomena in Sputtered Aluminum Planarization Processes.

M. A. Jones, J. A. Roberts, C. H. Ellenwood, M. W. Cresswell, and R. A. Allen. 1991, 6p Pub. in Proceedings of IEEE (Institute for Electrical and

Electronics Engineers) International Conference on Microelectronic Test Structures, Kyoto, Japan, March 18-20, 1991, v4 n1 p35-40.

Keywords: Very large scale integration, Scanning electron microscopy, Circuit interconnections, Chips(Electronics), Metallizing, Integrated circuits, Aluminum, Reprints, \*Test chips, Planarization.

A test chip has been designed and fabricated for the evaluation of surface-diffusion phenomena in sputtered aluminum planarization processes. It allows for confirmation of the correct sample cross-section bevel angle and orientation for scanning electron micro-scope (SEM) inspection of step coverage. These features eliminate ambiguities that may otherwise arise in the interpretation of the SEM images. The chip design provides arrays of vias with multiple combinations of size and spacing to enable characterization and mod-eling of the aluminum planarization phenomena for a full range of deposition parameters. It also incorporates electrically readable test structures that allow re-lating the SEM images of step coverage to corre-sponding electrical properties, such as electromigration, of the deposited metal. These are extracted from standardized electrical test structures designed and characterized for that purpose. The overall objective is to enable the selection of deposition parameters that simultaneously produce visually acceptable step-coverage images as well as optimized electrical properties

Not available NTIS
National Inst. of Standards and Technology (NEL),
Gaithersburg, MD. Semiconductor Electronics Div.
Knowledge Extraction Techniques for Expert
System Assisted Wafer Screening.
Final rept.
D. Khere M. W. C.

D. Khera, M. W. Cresswell, L. W. Linholm, G. Ramanathan, J. Buzzeo, and A. Nagarajan. 1990, 6p Pub. in Proceedings of International Semiconductor Manufacturing Science Symposium, Burlingame, CA., May 21-23, 1990, p44-49.

Keywords: \*Integrated circuits, Expert systems, Screening, Yield, Wafers, Reprints.

The paper describes a procedure for using induction-based classification techniques for identifying relationships between work-in-process (WIP) test structure data and future IC yield at wafer test on a wafer-by-wafer or lot-by-lot basis. The relationships are extracted from databases of previously processed WIP wafer test structure measurements and final wafer yield. They are presented in the form of rules relating WIP data to final yield. It is further shown that these rules, when incorporated into expert systems, can advise the human operator responsible for screening wafers which are likely to produce sub-marginal yield if processed to completion. These rules also identify the WIP test structure parameters and values which have historically provided the highest and lowest final wafer

PB92-116987 Not available NTIS
National Inst. of Standards and Technology (NEL),
Gaithersburg, MD. Semiconductor Electronics Div.
Assessment of Reliability Concerns for Wide-Temperature Operation of Semiconductor Devices and Circuits.

Final rept.

J. J. Kopanski, D. L. Blackburn, G. G. Harman, and D. W. Berning. 1991, 6p
Sponsored by National Aeronautics and Space Administration, Cleveland, OH. Lewis Research Center.

Pub. in Proceedings of International High Temperature Electronics Conference (1st), Albuquerque, NM., June 16-20, 1991, p137-142 1991.

\*Semiconductor \*Reliability(Electronics), Temperature effects, Arrhenius equation, High temperature, Accelerated tests, Circuits, Reprints.

Factors that may affect the long-term (30 yrs = approx 1 million h) reliability of electronic systems that can withstand temperature extremes (-150 to  $\pm$ 300 C) are

discussed. There is ample evidence that a straightforward application of the Arrhenius equation, with activa-tion energies determined from high-temperature accelreated stress testing, is not strictly valid for predicting real device lifetime. The relevance and validity of this traditional reliability assurance methodology, especially near the high-temperature operating limit, is critiqued. Some of the barriers to long-term reliable operation of devices and signific subject to extense the stress to long-term reliable operation of devices and signific subject to extense the stress to long-term reliable operations of devices and signific subject to extense the stress to long-term reliable operations of devices and signific subject to extense the stress to long-term reliable operations of devices and signific subject to extense the stress to long-term reliable operations of devices and significant subject to extense the stress to long-term reliable operations of the stress t ation of devices and circuits subject to extreme tem-peratures are identified in the broad areas of: (1) semiconductor materials, (2) components and circuit design, and (3) packaging and assembly. Finally, alter-native approaches to reliability assurance, not depend-ent on elevated temperature testing, which may be applicable to high-temperature electronics, are discussed.

100.826

PB92-117084 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Semiconductor Electronics Div. Persistent Photoconductivity in SIMOX Films. Final rept.

Final rept.

S. Mayo, J. R. Lowney, P. Roitman, and D. B.
Novotny. 1990, 2p
Contract DNA-IACRO-88-800
See also PB91-112409. Sponsored by Defense Nuclear Agency, Washington, DC.
Pub. in Proceedings of IEEE SOS/SOI Technology
Conference, Key West, FL., October 2-4, 1990, p156-

Keywords: \*Photoconductivity, Film resistors, Time dependence, Interfaces, Wafers, Reprints, \*SIMOX, SIMOX(Separation by IMplanted Oxygen), Photoinduced transient spectroscopy.

Photoinduced transient spectroscopy (PITS) was used to measure the persistent photoconductive (PPC) response in film resistors fabricated on two different commercial n-type SIMOX (Separation by IMplanted OXygen) wafers. A broadband, single-shot, flashlamp-pumped dye laser pulse was used to photoexcite interband electrons in the film, and the decay in the induced excess carrier population was measured at temperatures in the 60- to 220-K Range. The post-illumination conductivity transients observed show PPC signals exhibiting nonexponential character. They were recorded for periods of time up to 30 s at constant temperature. The photoconductive data from these film resistors are analyzed by using the Queisser and Theodorou potential barrier model, and a logarithmic time decay dependence is confirmed for the first time in SIMOX material. The sensitivity of PITS is demonstrated to be appropriate for characterization of the SIMOX interface structure and for material qualification.

100,827

PB92-117159

Not available NTIS
National Inst. of Standards and Technology (NEL),
Gaithersburg, MD. Semiconductor Electronics Div.
Band-Gap Narrowing and III-V Heterostructure
FFTs. FETs.

Final rept.

D. R. Myers, J. A. Lott, J. R. Lowney, J. F. Klem, and C. P. Tigges. 1990, 4p See also DE91000401.

Pub. in Proceedings of International Electron Devices Meeting, San Francisco, CA., December 9-12, 1990, p31.1.1-31.1.4.

Keywords: \*Field effect transistors, \*Energy gap, Aluminum gallium arsenides, Quantum wells, Valence bands, Reprints, Gallium indium arsenides, Density of states Heterostructures.

The authors calculate the magnitude of band-gap narrowing for GaAs-based alloys, and have included these results into one-dimensional heterojunction device models for strained In(0.15)Ga(0.85)As quantum-well MODulation-doped Field-Effect Transistors (MODFETs). Equivalent rigid shifts of as much as 102 meV are obtained for the valence band of depleted p-type Al(0.15)Ga(0.85) as doped as 5 x 10 to the 18th power/cc. Their simulations suggest that band-gap narrowing is most significant for p-channel MODFETs. The predicted effect of band-gap narrowing in p-channel MODFETs is the formation of parasitic conduction in the low-mobility parent dopant region. The parasitic conduction would reduce the intrinsic gain.

100.828

PB92-117217

Not available NTIS

# Semiconductor Devices

National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Precision Engineering Div.

Application of Transmission Electron Detection to X-ray Mask Calibrations and Inspection.

M. T. Postek, R. D. Larrabee, W. J. Keery, and E. Marx. 1991, 13p Pub. in Proceedings of SPIE (Society of Photo-Optical Instrumentation Engineers) - Integrated Circuit Metrology, Inspection, and Process Control V, v1464 p35-47 1991.

Keywords: \*Integrated circuits, \*Calibration, Transmission electron microscopy, Scanning electron microscopy, Electron detection, Dimensional measurement, Metrology, Inspection, Reprints, \*X ray masks, X ray lithography.

Masks used for the manufacture of integrated circuits by x-ray lithography can be calibrated and inspected in a scanning electron microscope by using the transmitted electron detection mode. By their nature, these masks present a measurement subject unique from most (if not all) other objects used in semiconductor processing because the support membrane is, by design, x-ray transparent. The characteristic can be used as an advantage in electron beam-based mask metrology since, depending upon the incident electron beam voltages, substrate composition and substrate thickness, the membrane can also be essentially electron transparent. The areas of the mask where the absorber structures are located are essentially x-ray opaque as well as electron opaque. Viewing the sample from a perspective below an x-ray mask can provide excellent electron signal contrast (depending upon the instrument conditions) between the absorber structure and the membrane. Thus, the mask can be viewed in the transmitted electron detection mode of the scanning electron microscope, and precise and potentially accurate dimensional measurements can be made.

100,829 PB92-117233 PB92-117233 Not available NTIS
National Inst. of Standards and Technology (NEL),
Gaithersburg, MD. Semiconductor Electronics Div.
Residual Defects in SIMOX: Threading Dislocations and Pipes.

Final rept.

P. Roitman, M. Edelstein, S. Krause, and S.

Visitserngtrukul. 1990, 2p Contract DNA-IACRO-88-800 Sponsored by Defense Nuclear Agency, Washington,

Pub. in Proceedings of IEEE SOS/SOI Technology Conference, Key West, FL., October 2-4, 1990, p154-

Keywords: \*Crystal defects, Crystal dislocations, Very large scale integration, Bipolar transistors, Stacking faults, Integrated circuits, Electron microscopy, Silicon, Reprints, \*SIMOX.

In the past few years, due to improved control of the ion implantation process and improved annealing sequences, a qualitative improvement has been realized in the structural quality of SIMOX films. The dense network of oxide precipitates and threading dislocations in the top silicon can be annealed out, reducing the dislocation density from about 10 to the 10th power/sq cm to about 100,000/sq cm or less. CMOS transistors and circuits have been successfully fabricated in this material. However, bipolar devices are sensitive to defect densities in this range, as is VLSI yield. Therefore, the defect density must be monitored and reduced. The authors discuss below some techniques for monitoring dislocations and stacking faults in SIMOX films. Also, a different type of defect, a silicon 'pipe' running through the buried oxide has been observed. The origin of these defects, and a technique for detecting them, will be described.

100,830 PB92-117241 Not available NTIS Notional Inst. of Standards and Technology (NEL), Gaithersburg, MD. Semiconductor Electronics Div. Round-Robin Study of Implants in Si and SiO2 by SIMS, RBS, and NAA.

Final rept.
P. Roitman, D. S. Simons, P. H. Chi, R. M. Lindstrom, G. E. Lux, S. Baumann, S. W. Novak, R. G. Wilson, D. Farrington, J. Keenan, F. A. Stevie, J. L. Moore, R. B. Inwin, A. J. Filo, C. W. Magee, R. Alcorn, and D. File. 1990, 3p

Pub. in Proceedings of International Conference on Secondary Ion Mass Spectrometry (SIMS VII) (7th), Monterey, CA., September 3-8, 1989, p115-117 1990.

Keywords: \*Ion implantation, \*Silicon dioxide, \*Silicon, Carbon, Sodium, Aluminum, Chromium, Iron, Copper, Reprints, Secondary ion mass spectroscopy

A round-robin study of implants of C, Na, Al, Cr, Fe, and Cu into Si and SiO2 has been conducted. The results are reported.

100.831

PB92-117282 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Semiconductor Electronics Div. Measurement, Use, and Interpretation of TCR.

H. A. Schafft. 1991, 7p Pub. in Proceedings of International Wafer Level Reliability Workshop, Lake Tahoe, CA., October 7-10, 1990, p211-217 1991.

Keywords: \*Integrated circuits, Stress testing, Electromigration, Metallizing Measurement, Reprints, \*Temperature coefficient of resistance.

A few comments are made about the measurement, use, and interpretation of the temperature coefficient of resistance (TCR). TCR is important when one wants to determine the temperature of a metallization line in an electromigraion stress test.

#### General

100,832

PB91-132241 PC A06/MF A01 National Inst. of Standards and Technology (NEL), Boulder, CO. Electromagnetic Fields Div.

Bibliography of the NIST Electromagnetic Fields Division Publications.

R. M. Lyons, and K. A. Gibson. Aug 90, 104p

NISTIR-3945

Supersedes PB90-163635.

Keywords: \*Electromagnetic fields, Electrical measurement, Dielectric properties, Electromagnetic inter-ference, Electromagnetic noise, Remote sensing, Radiation hazards, Antennas, Metrology, Wa Standards, Time domain, Near field, US NIST.

The bibliography lists the publications by the staff of the Electromagnetic Fields Division of the National Institute of Standards and Technology for the period January 1970 through July 1990. It supersedes PB90-163635 which listed the publications of the Electromagnetic Fields Division from January 1970 through magnetic Fields Division from January 1970 through August 1989. Topics covered include antennas, dielectric measurements, electromagnetic interference, microwave metrology, noise, remote sensing, time domain, and waveform metrology. Selected earlier publications from the Division's predecessor organizations. tions are included.

PB91-132266 PC A04/MF A01 National Inst. of Standards and Technology (NEL), Boulder, CO. Electromagnetic Technology Div. Metrology for Electromagnetic Technology: A Bib-liography of NIST Publications. M. E. DeWeese. Aug 90, 66p NISTIR-3946 Supersedes PB90-161670.

Keywords: \*Metrology, \*Bibliographies, Optical communication, Superconductors, Electrooptics, Cryogenics, Lasers, \*Electromagnetic metrology, Cryoelectronics, Optical fibers, Superconducting devices, US

The bibliography lists the publications of the personnel of the Electromagnetic Technology Division of NIST during the period from January 1970 through publication of this report. Topics include cryoelectronics, electromagnetic metrology, lasers, magnetics, optical fibers, and superconducting materials. A few earlier references that are directly related to the present work of the Division are also included.

100.834

PB91-133868 Not available NTIS National Inst. of Standards and Technology (NEL), Boulder, CO. Electromagnetic Technology Div. Eddy Current Probe Characterization Using an Impedance Plane Display Instrument. Final rept.

T. E. Capobianco. 1989, 9p

Sponsored by Army Materials Technology Lab., Watertown, MA.

Pub. in Proceedings of Defense Conference on Nondestructive Testing (38th), San Antonio, TX., October 31-November 2, 1989, p193-201.

Keywords: \*Eddy current tests, \*Electrical impedance, \*Standards, Display devices, Nondestructive tests, Electromagnetic testing, Calibrating, Conductivity, Alu-minum alloys, Probes, Reprints, \*Calibration.

The U.S. Army is sponsoring work at the National Institute of Standards and Technology to develop a military standard for characterizing eddy current probe performance. Presently, the test method of this draft standard is the measurement of the probe impedance change when the probe is applied to test blocks of two different conductivities. The authors hoped that this impedance measurement would be easy to perform in the field, but they discovered that field and depot level operations lack the equipment for measuring imped-ance. This has become a serious obstacle to the implementation of the standard. However, depot operations often have an eddy current instrument which displays flaw signals in the impedance plane. These instruments do not display the actual impedance values of the flaw signals presented but could possibly be calibrated for this purpose. Results of an experiment where a calibration technique was tried and eddy current probe impedances measured are presented.

100.835

PB91-134213 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Electricity Div.

Transition from Trichel-Pulse Corona to Dielectric

Barrier Discharge.

Final rept.

S. V. Kulkarni, R. J. Van Brunt, and V. K. Lakdawala. 1990, 8p

Sponsored by Department of Energy, Washington, DC.

Div. of Electric Energy Systems.

Pub. in Proceedings of Annual Report Conference on Electrical Insulation and Dielectric Phenomena, Pocono Manor, PA., October 28-31, 1990, p267-274.

Keywords: Electrical insulation, Electric discharges, Dielectrics, Reprints, \*Corona discharges, Trichel pulses.

Experiments are conducted to investigate the conditions under which the transition from negative corona to dielectric barrier controlled discharge occurs. A negative point-plane electrode (covered with PTFE dielecative point-plane electrode (covered with FTE defective) geometry is studied using a newly developed partial discharge detection technique. At a critical gapdistance, an abrupt transition from a rapid pulsating behavior to a widely distributed random pulse behavior is observed. The critical distance increases with increasing diameter of the solid dielectric and decreases with increase in applied voltage. The influence of dielectric surface charging on the Trichel pulse behavior is manifested by the measured pulse height and time separation distributions. As the influence of dielectric charging increases, the pulse separation distribution begins to broaden significantly and the corresponding pulse height distribution becomes narrower.

100,836 PB91-134528 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Electricity Div. Collisional Electron-Detachment and Ion-Conver-

sion Processes In SF6. Final rept.

J. K. Olthoff, R. J. Van Brunt, Y. Wang, L. D. Doverspike, and R. L. Champion. 1990, 16p Sponsored by Department of Energy, Washington, DC. Pub. in Nonequilibrium Effects in Ion and Electron Transport, p229-244 1990.

Keywords: \*Sulfur hexafluoride, Electric discharges, Cross sections, Reprints, \*Electron detachment, \*Ionmolecule collisions, Fluorine ions, Sulfur fluorides.

Results are summarized from the first direct measurements of absolute cross sections for electron-detachment and ion-conversion processes involving interactions of SF6(1-), SF5(1-) and F(1-), with SF6. These cross sections are used to calculate electron-detachment and ion-conversion reaction coefficients as func-

#### General

tions of electric field-to-gas density ratios (E/N) for various reactions. The relevance of these results is discussed to the interpretation of data from uniformfield drift-tube measurements and measurements of electrical-discharge initiation processes.

100,837 PB91-134684

Not available NTIS National Inst. of Standards and Technology (NEL),

Gaithersburg, MD. Electricity Div.
Electrical Breakdown and Streamer Statistics in Nhexane under Uniform Field Conditions.

Final rept. K. L. Stricklett, E. F. Kelley, H. Yamashita, H. Kawai,

and C. Fenimore. 1990, 4p
Sponsored by Department of Energy, Washington, DC.
Office of Energy Storage and Distribution.
Pub. in Proceedings of IEEE (Institute of Electrical and

Electronics Engineers) International Symposium on Electrical Insulation, Toronto, Canada, June 3-6, 1990,

Keywords: \*Hexanes, \*Dielectric breakdown, \*Electric discharges, High speed photography, Liquids, Reprints, \*Breakdown(Electronic threshold), Streamer initiation.

Under uniform field conditions, two modes of electrical breakdown are observed in liquid n-hexane: break-down may be initiated by either cathode or anode streamers. This observation suggests that two unique sets of phenomena lead to electrical breakdown. In the work described, high-speed photography is employed to obtain a record of each breakdown event thereby providing statistical information regarding the relative frequencies of anode and cathode processes. The degree to which the relative probability for either process is influenced by experimental conditions is discussed.

PB91-134916 Not available NTIS National Inst. of Standards and Technology (NEL), Boulder, CO. Electromagnetic Fields Div.

Dual Six-Port Reflectometer Systems Using Wave-

guide in the Frequency Range 18-50 GHz.
Final rept.
C. M. Weil, F. E. Marler, J. R. Major, M. F. Weidman, and D. H. Russell. 1989, 13p
Pub. in ARFTG Conference Digest (33rd), Long Beach, CA., June 15-16, 1989, p76-88.

Keywords: \*Microwave reflectometers, Extremely high frequencies, Superhigh frequencies, Millimeter waves, Waveguides, Scattering, Bolometers, Reprints, Six port, Uncertainty.

The development and evaluation of three dual six-port reflectometer systems, that use WR-42, WR-28 and WR-22 waveguides are discussed; these cover the frequency range 18-50 GHz. The systems are capable of automated or semiautomated operation and will provide complex scattering parameter data for customer waveguide components, as well as effective efficiency data for power sensors. Some representative measurement data are presented that demonstrate that these systems yield results that do not differ significantly from those obtained using older measurement systems. Some discussion of measurement uncertainties is also included.

100,839 PB91-135020 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Electricity Div. Effect of High Pressure on Prebreakdown Phe-

nomena in n-Hexane.

Final rept. H. Yamashita, H. Kawai, K. L. Stricklett, and E. F. Kelley. 1990, 6p

Sponsored by Department of Energy, Washington, DC. Pub. in Proceedings of International Conference on Conduction and Breakdown in Dielectric Liquids (10th), Grenoble, France, September 10-14, 1990, p404-409.

Keywords: \*Dielectric breakdown, \*Electric discharges, Liquids, Electric fields, Electric potential, Shadowgraph photography, Reprints, \*Pressure effects, \*Hexane, Nonuniform fields, Streamer initiation.

The effect of pressure on the initiation of prebreakdown streamers in a-hexane in a non-uniform field is investigated. Using a high-magnification (100x) highresolution (1 micrometers) optical system and a high-speed camera, the initial growth of low-density streamers propagating from a needle cathode is examined at pressures ranging from 0.1 to 1.1 MPa. The initial streamer is a single filament which grows to approximately 4 micrometers in diameter and 8 micrometers in length before the appearance of a dense bushy structure at its tip. Oscillatory behavior of the initial streamer is observed in which the diameter of the intitial streamer expands and contracts as the streamer grows. The pressure dependence of the streamer initiation voltage is shown.

100,840 PB91-147223 PB91-147223 Not available NTIS National Inst. of Standards and Technology (NEL), Boulder, CO. Electromagnetic Technology Div. High Speed Magnetic Field Sensors Based on Iron Garnets. Garnets.

Final rept M. N. Deeter, A. H. Rose, and G. W. Day. 1990, 2p Pub. in Proceedings of AFCEA Department of Defense Fiber Optics Conference, McLean, VA., March 20-23, 1990, p423-424.

Keywords: \*Yttrium iron garnets, \*Magnetic measurement, \*Magnetic fields, \*Magnetooptics, Faraday effect, Optical fibers, Fiber optics, Sensors, Reprints.

The authors characterize magnetic field sensors based on the Faraday effect in ferrimagnetic iron gar-nets in terms of their sensitivity and frequency response. Signal-to-noise measurements at 80 Hz on a sample of yttrium iron garnet yield noise equivalent magnetic fields of 10 nT/ Hz. Frequency response measurements exhibit virtually flat response to approximately 700 MHz.

100,841 PB91-147702 Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Precision Engineering Div.

Determination of Fields Near a Silver Strip on a Glass Substrate. Final rept.

E. Marx, and E. C. Teague. 1988, 9p

Pub. in Proceedings of SPIE (Society of Photo-Optical Instrumentation Engineers) - Scanning Microscopy Technologies and Applications, v897 p176-184 1988.

Keywords: \*Dimensional measurement, \*Light scattering, Electromagnetic scattering, Optical scanning, Integral equations, Resonance scattering, Near field, Reprints, \*Silver strips.

The theory and numerical considerations that are used in the computation of the scattered electromagnetic fields near the surface of a silver strip on a glass substrate are presented. These calculations provide theoretical guidance for the measurement of the width of the strip by means of near-field optical scanning. The dimensions of the strip cross section, e.g. 300 nm by 100 nm, can be a fraction of the wavelength of the incident light, 632.8 nm. The flux 1 nm above the surface shows sharp spikes at the edges of the strip. The features of the fields near such a surface could be used for accurate determination of the width of the strip by measurements up to about 30 nm above the strip. The effects of other variables are also shown in the figures.

PB91-148676 Not available NTIS National Inst. of Standards and Technology (NEL), Boulder, CO. Electromagnetic Technology Div. Integrity Tests for High-(T sub c) and Conventional Critical-Current Measurement Systems. Final rept.

Fillal rept.
L. F. Goodrich, and S. L. Bray. 1990, 8p
Sponsored by Department of Energy, Washington, DC.
Pub. in Advances in Cryogenic Engineering (Materials), v36 ptA p43-50 1990.

Keywords: \*Critical current, High temperature super-conductors, Electrical measurement, Power supplies, Test methods, Voltmeters, Reprints, Ground loops.

Critical-current measurement systems must be extremely sensitive to the small differential voltage that is present across the test specimen as it changes from the zero resistance state to the flux-flow resistance state. Consequently, these measurement systems are also sensitive to interfering voltages. Such voltages can be caused by ground loops and by common mode voltages. Specific methods for testing the sensitivity of critical-current measurement systems and for detecting the presence of interfering voltages are discussed. These include a simple procedure that simulates the

zero resistance state and the use of an electronic circuit that simulates the flux-flow resistance state.

100.843

PB91-158816 Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Chemical Process Metrology Div.
Surface Acoustical Wave Spectroscopy for High

**Humidity Sensing.** 

Final rept.
P. H. Huang. 1987, 5p
Pub. in Proceedings of International Conference on Solid-State Sensors and Actuators (4th), Tokyo, Japan, June 2-5, 1987, p462-466.

Keywords: \*Surface acoustic wave devices, \*Humidity measurement, High humidity, Lithium niobates, Electric fields, Acoustic fields, Sensors, Reprints, \*SAW devices.

Polar water molecules in ambient moist air can be made to interact with the electric and acoustic fields of surface acoustical waves(SAW) in plezoelectric crystal surface. The interaction causes a change in the amplitude of the received surface wave which is proportional to the energy density of the wave. An amplitude-modulated SAW technique, which does not use adsorptive coatings, has been used to study this electroacoustic interaction for high humidity sensing in the range 90 to 98% RH. The sensor system consists of two identical high frequency, wide band SAW delay lines. One is used as a reference channel with shorted electric fields at the surface. The reference delay line is maintained in an environment of nearly zero percent relative humidity. The ratio of voltage output from the sensing channel to that of the reference channel has been measured. An exponential relationship exists between the measured voltage ratio and the relative humidity in the range from 89 to 98% for SAW frequencies at 210, 220, 230, 240, and 250 MHz, respectively. Measurements of spectral group delay reveal the limitation on the transmission bandwidths of the sensor system for high humidity sensing.

100.844 PB91-161919 Not available NTIS National Inst. of Standards and Technology (NEL),

Boulder, CO. Electromagnetic Fields Div.
Improved Technique for Determining Complex
Permittivity with the Transmission/Reflection Method.

Final rept J. Baker-Jarvis, E. J. Vanzura, and W. A. Kissick.

1990, 8p
Pub. in IEEE (Institute of Electrical and Electronics Engineers) Transactions on Microwave Theory and Techniques 38, n8 p1096-1103 Aug 90.

Keywords: \*Permittivity, Dielectric properties, Permeability, Transmission, Reflection, Reprints.

The transmission/reflection method for complex permittivity and permeability determination is studied. The special case of permittivity measurement is examined in detail. New robust algorithms for permittivity determination that eliminate the ill-behaved nature of the commonly used procedures at frequencies corresponding to integer multiples of one-half wavelength in the sample are presented. An error analysis is presented which yields estimates of the errors incurred due to the uncertainty in scattering parameters, length measurement, and reference plane position. In addition, new equations are derived for determining complex permittivity independent of reference plane position and sample length.

100,845 PB91-161992 Not available NTIS National Inst. of Standards and Technology (NEL),

National Inst. of Standards and Technology (NEL), Boulder, CO. Electromagnetic Fields Div. TEM/Reverberating Chamber Design/Concept Study: A Single Facility for Large System Radiated EMC Testing, 10 kHz - 40 Ghz.

Final rept.

M. L. Crawford. 1989, 15p Pub. in Proceedings of EMC EXPO Conference Record, Washington, DC., August 1-3, 1989, 15p.

Keywords: \*Reverberation chambers, \*Electromagnetic compatibility, Transmission lines, Scale models, Performance, Design, Reprints, US NIST.

The paper describes work in progress at NIST to develop a single, integrated facility using a large shielded enclosure configured as a TEM transmission line

driven reverberating chamber. TEM test fields are generated at frequencies below multimode cutoff, and mode-stirred test fields are generated at frequencies above multimode cutoff. The paper discusses a proposed facility design, advantages and limitations, the theoretical basis for the work, and the proposed experimental approach for evaluating a 1/10 scale model of a large enclosure having a test volume of 8m x 16m x 30m

100,846 PB91-162362 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Electricity Div. Cutting the High Cost of Testing.

T. M. Souders, and G. N. Stenbakken. 1991, 4p Pub. in IEEE (Institute of Electrical and Electronics Engineers) Spectrum, p48-51 Mar 91.

Keywords: \*Test methods, Computer applications, Analog circuits, Linear equations, Mathematical Analog circuits, models, Reprints.

An approach is presented for optimizing the testing of analog and mixed-signal devices. The entire process is performed with algebraic operations on an appropriate model. The paper demonstrates how this is accomplished, using simple calls with public-domain software. Examples of test results achieved using this approach are included.

PB91-162370 Not available NTIS National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Fields Div.
Intercomparison of NBS Noise Calibration Serv-

ices.

D. F. Wait, W. C. Daywitt, and G. Counas. 1988, 2p Pub. in Proceedings of Conference on Precision Elec-tromagnetic Measurements 'CPEM '88 Digest', Tsu-kuba, Ibaraki, Japan, June 7-10, 1988, p209-210.

Keywords: \*Thermal noise, \*Standards, Microwave radiometers, Noise temperature, Reflectometers, Calibration, Reprints, Intercomparison.

New, less restrictive thermal noise calibration services recently established in the frequency range of 2 - 12.4 GHz overlap prior NBS services and provide an opportunity for intercomparison. The agreement between old and new calibration systems is better than 0.4%.

100,848 PB91-171959 PC A08/MF A01 National Inst. of Standards and Technology (NEL), Boulder, CO. Electromagnetic Fields Div.

Transmission/Reflection and Short-Circuit Line

Permittivity Measurements. Technical note.

J. Baker-Jarvis. Jul 90, 156p NIST/TN-1341 Also available from Supt. of Docs. as SN003-003-

Keywords: \*Dielectric properties, Microwaves, Electrical measurement, Calibration, Permeability, Reflection, Uncertainty, Coaxial cables, Computer programs, \*Permittivity measurement, Loss factors

The transmission/reflection and short-circuit line methods for measuring complex permittivity are examined. Equations for permittivity are developed from first principles. New robust algorithms that eliminate the illbehaved nature of the commonly used transmission/ reflection method at frequencies corresponding to in-tegral multiples of one-half wavelength in the sample are presented. These allow measurements to be made on samples of any length. An uncertainty analysis is presented which yields estimates of the errors incurred due to the uncertainty in scattering parameters, length measurement and reference plane position. The equations derived here indicate that the minimum uncertainty for transmission/reflection measurements of nonmagnetic materials occurs at integral multiples of one-half wavelength in the material. In addition, new equations for determining complex permittivity independent of reference plane position and sample length are derived. New equations are derived for permittivity determination using the short-circuit line allow positioning the sample arbitrarily in the sample holder.

100,849 PB91-175240 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Electrosystems Div. Recent Developments in Digital Oscilloscopes.

Final rept. H. K. Schoenwetter. 1989, 2p Pub. in Proceedings of IEEE (Institute of Electrical and Electronics Engineers) Instrumentation and Measurement Technology Conference, Washington, DC., April 25-27, 1989, p154-155.

Keywords: \*Oscilloscopes, Digitizers, Reprints, \*Digital oscilloscopes, Waveform recorders.

The paper reviews the latest developments in digital storage oscilloscopes (DSOs) as reported in the open literature. DSOs are used to digitize and store waveforms which may be compared, analyzed, and manipulated. DSO capabilities usually include programmability, automatic waveform parameter measurement, the display of pre-trigger signal activity, and waveform averaging to reduce noise and ripple.

Not available NTIS PB91-175356 National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Fields Div.

Lattice Approach to Environments Irradiated by Unknown Sources.

Final rept.

J. Randa, and M. Kanda. 1987, 5p

Pub. in Proceedings of the International Zurich Symposium and Technical Exhibition on Electromagnetic Compatibility (7th), Zurich, March 3-5, 1987, p191-195.

Keywords: \*Electromagnetic environments, Maxwells equations, Numerical solution, Reprints, Successive overrelaxation method, III posed problems.

An approach is suggested to the characterization of electromagnetic environments irradiated by unknown sources. The approach is based on the numerical solution of Maxwell's equations subject to the constraints imposed by the measured values of the field at a small number of measurement points and by boundary conditions. The idea is demonstrated using a particular method for the numerical solution. Examples which demonstrate the approach but reveal deficiencies in the numerical method are given. Possible future directions are suggested.

100.851

PB91-175398 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Electricity Div.

Measurements of Power Frequency Magnetic

Fields Away from Power Lines.

M. Misakian, J. M. Silva, and R. S. Baishiki. 1991,

Pub. in IEEE (Institute of Electrical and Electronics Engineers) Transactions on Power Delivery 6, n2 p901-911 Apr 91.

Keywords: \*Magnetic fields, Residential buildings, Industrial buildings, Environments, Measurement, Calibration, Reprints.

Recent epidemiological studies have focused attention on the measurement of ambient level power frequency magnetic fields in residential and industrial set-tings. These fields can be as much as two orders of magnitude smaller than power line magnetic fields and can also contain significant levels of harmonic content. Because the existing IEEE standard for characterizing power frequency magnetic fields is intended for measurements near power lines, it has a number of inadequacies if used alone for guidance during the measurement of residential fields. The paper describes the instrumentation, calibration procedures, and outlines measurement strategies which can overcome some of the shortcomings of the existing standard. Examples of ambient level magnetic field measurements are also

PB91-184754 PC A03/MF A01 National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Center for Electronics and Electrical Engineering.

Center for Electronics and Electrical Engineering Technical Publication Announcements Covering Center Programs, July to September 1990, with 1991 CEEE Events Calendar. J. A. Gonzalez, Apr 91, 31p NISTIR-4537

See also PB90-206491.

Keywords: \*Semiconductor devices, \*Metrology, Electrical engineering, Electronics, Electromagnetic inter-

ference, Integrated circuits, Antennas, Optical fibers, Signal processing, Sensors, Waveforms, Electrooptics, Photodetectors, High temperature superconductors, Progress report.

This is the twenty-sixth issue of a quarterly publication providing information on the technical work of the National Institute of Standards and Technology (formerly the National Bureau of Standards) Center for Electronics and Electrical Engineering. This issue of the CEEE Technical Publication Announcement covers the third quarter of calendar year 1990. Topics discussed include the following: Semiconductor Technology Program; Signals & Systems Metrology Program; Fast Signal Acquisition Processing & Transmission; Fast Signal Acquisition, Processing, & Transmission; Electrical Systems; Electromagnetic Interference; 1991 CEEE Calendar.

100.853

PB91-189290 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Electricity Div. Measurement Reliability: The Detection of Nonlin-

earities.

Final rept.

C. P. Fenimore, and G. J. FitzPatrick. 1991, 6p Sponsored by Defense Nuclear Agency, Washington,

Pub. in Proceedings of Space Nuclear Power Systems Symposium (8th), Albuquerque, NM., January 7-10, 1991, p1113-1118.

\*Electrical measurement, Keywords: Spacecraft Reliability(Electronics), supplies. power Failure(Electronics), Photomultiplier tubes, Voltage dividers, Kerr cells, Error analysis, Reprints.

The detection of a single measurement failure in a compound measurement system consisting of a voltage divider and a Kerr cell is demonstrated. The comparison of measurement devices based on distinct technologies is inherently robust; they may be expected to have distinct failure characteristics. The Kerr comparison is based on model fitting applied to numerically-generated data and experimental, digitallyrecorded waveforms. The characteristic signatures of two measurement errors are found: for a quadratic nonlinearity in the detector and for an overdriven photodetector. The length of the data records permits the detection of nonlinearities which are comparable to the noise in magnitude. Detection of such errors is a prerequisite to recalibration in software which enables error correction in remote applications, such as space power systems.

100,854

PB91-189308 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Electricity Div.
Incompatibility between the 100/1300 Surge Test
and Varistor Failure Rates.

Final rept.

C. P. Fenimore, and F. D. Martzloff, 1991, 6p Pub. in Proceedings of International Zurich Symposium (9th), and Technical Exhibition on Electromagnetic Compatibility, Zurich, Switzerland, March 12-14, 1991, n525-530

Keywords: \*Surges, \*Varistors, Mathematical models, Nonlinear systems, Circuits, Tests, Reprints.

A proposed high-energy surge test featuring a 100/ 1300 microsec waveform and a peak voltage of 2.3 times the peak voltage of the low-frequency mains is under consideration by the IEC. The energy storage capacitor suggested for the surge generator, originally specified as high as 25 000 microfared, has been scaled down but is still at a level of several thousand microfarads. To determine the energy dissipated in various surge tests, numerical integration is applied to a simple but realistic mathematical model of a test circuit. The energy that would be deposited into a varistor of the voltage rating commonly used in protecting load equipment, if subjected to this test, far exceeds the ca-pability of the varistor, but reported varistor failure rates do not reflect such a situation. Thus, a re-examination of the premises that led to the 100/1300 microsec test specifications appears necessary

100.855

PB91-189811 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Electricity Div.

#### **ELECTROTECHNOLOGY**

#### General

Real, Realistic Ring Waves for Surge Testing.

Final rept. F. D. Martzloff, and G. Pellegrini. 1991, 6p Pub. in Proceedings of the International Zurich Symposium and Technical Exhibition on Electromagnetic Compatibility (9th), Zurich, Switzerland, March 12-14, 1991, p499-504.

Keywords: \*Surges, Data transmission systems, Transmission lines, Power lines, Lightning, Transients, Test methods, Reprints, Ring waves.

Five independent investigations on the coupling of surges into low-voltage circuits (data or power lines), and of their effects, show that a damped oscillatory transient is a real, realistic stress for equipment connected to these lines.

100,856 PB91-202895 Not available NTIS National Bureau of Standards (NEL), Boulder, CO.

Electromagnetic Fields Div.
TEM Driven Reverberating Chamber, a Single Facility for Radiated EMS/V Testing, 10 kHz - 18 GHz.

M. L. Crawford. 1987, 11p
Pub. in Proceedings of International Conference on Electromagnetic Compatibility EMC EXPO 87, San Diego, CA., May 19-21, 1987, pT11.18-T11.28.

Keywords: \*Reverberation chambers, \*Electromagnetic testing, Electromagnetic susceptibility, Vulnerability, Test facilities, Performance evaluation, Operation, Design, Reprints.

The paper discusses the design, operation, and evaluation of a reverberating chamber, excited by a transverse electromagnetic (TEM) transmission line, for use in establishing radiated electromagnetic fields for susceptibility/vulnerability (EMS/V) testing of electronic equipment. The potential range of application is from 10 kHz to 18 GHz. Included are brief descriptions of the facility, the operation procedures, the methodfor determining the test field amplitude inside the chamber, and the evaluation of the chambers electrical parameters such as VSWR and E-field strength as a function of input power. Also the E-field spatial uniformity and a summary of measurement uncertainties and conclusions derived from the test results are pre-

100,857 PB91-203885 Not available NTIS National Inst. of Standards and Technology (NEL), Boulder, CO. Electromagnetic Fields Div.
Simultaneous versus Independent Injection Testing of Nonlinear Multiport Systems.

Final rept.

J. Randa. 1991, 4p

Pub. in Proceedings of International Zurich Symposium and Technical Exhibition on Electromagnetic Compatibility (9th), Zurich, Switzerland, March 12-14, 1991,

Keywords: \*Electromagnetic susceptibility, Electromagnetic interference, Nonlinear systems, Reprints,

The paper is a theoretical investigation of the question whether, in injection testing of a multiport system, all ports must be injected and tested simultaneously. A general, nonlinear, three-port system is analyzed. Conditions under which the ports can be tested separately are derived, and problems with the practical applica-tion of these conditions are pointed out. Systems with memory are also treated, and the extension to general multiports is given. The relevance to bulk injection testing is discussed.

100,858 PB91-236844 Not available NTIS National Inst. of Standards and Technology (EEEL), Roulder, CO. Electromagnetic Fields Div.
Improved Technique for Measuring Permittivity of
Thin Dielectrics with a Cylindrical Resonant Cavity. Final rept.

M. D. Janezic, and J. H. Grosvenor. 1991, 5p Sponsored by Department of the Navy, Washington,

Pub. in Proceedings of IEEE (Institute of Electrical and Electronics Engineers) Instrumentation and Measurement Technology Conference Enhancing Productivity with Instrumentation and Measurement Technologies, Atlanta, GA., May 14-16, 1991, p580-584.

Keywords: \*Dielectrics, \*Permittivity, Electrical measurement, Dielectric properties, Cavity resonators, Alu-

minum oxide, Magnesium titanates, Polystyrene, Microwaves, Reprints.

A new technique for measuring the relative permittivity of thin, low-loss dielectric materials in a cylindrical resonant cavity has been developed. A thin dielectric sample, of unknown characteristics, is placed upon a thicker dielectric sample whose permittivity is well characterized. Both samples are then placed on the endplate in the cylindrical resonant cavity. In this way, the thin sample is placed in a region of the cavity where interaction with the electromagnetic fields is greater. From knowledge of the cavity's resonant frequency, dimensions of the cavity and both dielectric samples, and the permittivity of the thicker sample, the authors are able to use iterative techniques to accurately determine the permittivity of the thin dielectric sample. A derivation and discussion of the theory used in this layered-dielectric permittivity measurement technique is provided. Also, measurement results, at frequencies between 9 and 10 GHz, are given.

100,859 PB91-237214 PB91-237214 Not available NTIS
National Inst. of Standards and Technology (EEEL),
Gaithersburg, MD. Electricity Div.
Precision Qualification of Watthour Meters.
Final rect. Final rept.

J. D. Ramboz, C. Fenimore, and S. B. Schiller. 1991,

Pub. in IEEE (Institute of Electrical and Electronics Engineers) Transactions on Instruments and Measurement 40, n2 p406-409 Apr 91.

Keywords: \*Watt hour meters, Electric energy meters, Experimental design, Electrical measurement, Precision, Standards, Reprints.

One of the NIST Measurement Assurance Programs transfers the unit of the watthour using transport meters. For the application, the response of these meters to variations in environmental conditions must be well-characterized. A statistically planned experi-ment is employed to determine corrections for the response of each meter to varying conditions of voltage, current, temperature, and power factor. This qualifica-tion procedure is designed to be efficient with the number of test points and to yeild estimates of the model parameters describing the corrections.

Not available NTIS PB91-237222 National Inst. of Standards and Technology (NEL), Boulder, CO. Electromagnetic Fields Div.

Theoretical Considerations for a Thermo-Optic Microwave Electric-Field-Strength Probe.

Final rept. J. Randa, 1990, 8p

Sponsored by Naval Ocean Systems Center, San

Pub. in Jnl. of Microwave Power and Electromagnetic Energy 25, n3 p133-140 1990.

Keywords: \*Electric fields, \*Probes(Electromagnetic), Microwave equipment, Electrical measurement, Ultra-high frequency, Superhigh frequency, Millimeter waves, Reprints.

Theoretical background for the design of a microwave electric-field probe is presented. The design uses a fiberoptic thermometer to measure the temperature rise of a resistive sphere or spherical shell in an electroot a resistive sphere or spherical shell in an electro-magnetic field. Design parameters are chosen to opti-mize sensitivity and frequency response for the 1 GHz to 10 GHz range. These parameters also result in good frequency response well into the millimeter-wave range. Advantages of the design are that it is small, nonpertubing, and can be used in high electromagnet-ic fields.

100,861 PB91-237644 Not available NTIS National Inst. of Standards and Technology (EEEL), Gaithersburg, MD. Electricity Div.
Influence of Memory Propagation on Phase-Re-

solved Stochastic Behavior of AC-Generated Partial Discharges.

Final rept. R. J. Van Brunt, and E. W. Cernyar. 1991, 3p Sponsored by Department of Energy, Washington, DC. Office of Energy Storage and Distribution. Pub. in Applied Physics Letters 58, n23 p2628-2630, 10 Jun 91

Keywords: \*Electric discharges, Stochastic processes, Static electricity, Alternating current, Dielectrics, Reprints.

Using measurements of phase-restricted conditional partial-discharge pulse-amplitude and phase distribu-tions, it is shown for the first time that the stochastic properties of a dielectric-barrier type of partial discharge generated by an ac voltage are significantly influenced by memory associated with charge deposited on the dielectric surface by preceding discharge events. The memory effect must be considered in any attempt to interpret results of phase-resolved partialdischarge measurements.

100.862

PB91-237776 Not available NTIS National Inst. of Standards and Technology (EEEL), Boulder, CO. Electromagnetic Fields Div. Translate LRL and LRM Calibrations. Final rept.

D. Williams, R. Marks, and K. Phillips. 1991, 5p Pub. in Microwaves and RF 30, n2 p78, 80-82 and 84, Feb 91.

Keywords: \*Calibration, Probes(Electromagnetic), Microwaves, Wafers, Reprints, LRM method, LRL method, Line reflect match method, Line reflect line method. Automatic network analyzers.

The Line-Reflect-Match calibration technique (LRM) is reviewed. Unless the match standard is perfect, cali-bration using the most common form of LRM differs from that of the Line-Reflect-Line technique (LRL). The authors present an explicit transformation which relates the two calibrations.

PD A03/MF A01
National Inst. of Standards and Technology (NEL),
Gaithersburg, MD. Center for Electronics and Electrical Engineering.

Center for Electronics and Electrical Engineering Technical Publication Announcements Covering Center Programs, October to December 1990, with

1991 CEEE Events Calendar.
J. A. Gonzales. Aug 91, 32p NISTIR-4645
See also PB90-265232 and PB91-184754.

Keywords: \*Electrical engineering, \*Electronics, Semiconductors(Materials), Metrology, Signal processing, Electromagnetic interference, Antennas, Lasers, Magnetic materials, Microwaves, Fiber optics, Superconductors, Electrooptics, Abstracts, Technology innovation, Semiconductor devices, NIST(National Institute of Standards and Technology), CEEE(Center for Electronics and Electrical Engineering).

This is the twenty-seventh issue of a quarterly publication providing information on the technical work of the National Institute of Standards and Technology (for-National Institute of Standards and Technology (formerly the National Bureau of Standards) Center for Electronics and Electrical Engineering. The issue of the Center for Electronics and Electrical Engineering Technical Publication Announcements covers the fourth quarter of calendar year 1990. Abstracts are provided by technical area for papers published this quarter. quarter.

100.864

PB92-112309 National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Semiconductor Electronics Div. Electronics and Electrical Engineering Laboratory Technical Publication Announcements Covering

Laboratory Programs, January to March 1991, with 1991 EEEL Events Calendar.
J. A. Gonzalez. Sep 91, 20p NISTIR-4675 See also PB91-240838.

Keywords: "Electromagnetic interference, "Microelectronics, "Electrooptics, "Metrology, Integrated circuits, Bipolar transistors, High temperature superconductors, Signal processing, Millimeter waves, Antennas, Lasers, Microwaves, Optical fibers, Magnetic materials, Sensors, Fiber optics, Progress report, Abstracts.

The report is the twenty-eighth issue of a quarterly publication providing information on the technical work of the National Institute of Standards and Technology, Electronics and Electrical Engineering Laboratory. The issue of the EEEL Technical Publication Announcements covers the first quarter of calendar year 1991. Abstracts are provided by technical area for papers published this quarter. Major topic areas include the following: Semiconductor microelectronics; Signal acquisition, processing, and transmission; Electrical systems. tems; Electromagnetic interference.

100,865 PB92-112325 PC A03/MF A01 National Inst. of Standards and Technology, Boulder,

Optimization Techniques for Permittivity and Permeability Determination.
P. D. Domich, J. Baker-Jarvis, and R. G. Geyer. Jun

91, 23p NISTIR-4571

Keywords: \*Permeability, \*Permittivity, Regression analysis, Complex variables, S matrix, Optimization, Microwaves, Transmission lines, Glass, Yttrium iron garnets, Barium titanates, Nickel ferrite, Polystyrene, Polymers.

The paper discusses optimization techniques for the determination of complex permittivity and permeability in transmission lines. The traditional theoretical model using scattering parameters is extended into a mathematical regression model that can be solved with widely accepted numerical techniques. The new model produces accurate primary mode results for the samples tested including nonmagnetic materials with high dielectric constants. An extension of the model includes responses due to higher order modes. The general model determines parameters to specify the spectral functional form of complex permittivity and permeability and is capable of small corrections to independent variable data including angular frequency, sample length, sample position, and cutoff wavelength. The method provides reliable determination for both low and high permittivity materials.

100.866 PB92-116367 PC A06/MF A02
National Inst. of Standards and Technology (EEEL),
Boulder, CO. Electromagnetic Technology Div.
Bibliography of the NIST Electromagnetic Fields
Division Publications.
R. M. Lyons, and K. A. Gibson. Aug 91, 108p
NISTIR-3973
Supersedes PR04-40044 PC A06/MF A02

Supersedes PB91-132241.

Keywords: \*Electromagnetic fields, \*Bibliographies, Electrical measurement, Dielectric properties, Electromagnetic interference, Electromagnetic noise, Remote sensing, Time domain, Radiation hazards, Near field, Antennas, Metrology, Waveforms, Stand-ards, Microwaves, Attenuation, Dielectric measureards, Microwaves, Attenuation, Dielectric measure-ments, Microwave metrology, Microwave power, Im-pedance, Near-field antenna measurements, Noise, Nonionizing radiation, Waveform metrology.

The bibliography lists the publications by the staff of the Electromagnetic Fields Division of the National Institute of Standards and Techology for the period Jan-uary 1970 through July 1991. It supersedes NISTIR 3945, which listed the publications of the Electromagnetic Fields Division from January 1970 through July 1990. Selected earlier publications from the Division's predecessor organizations are included.

100,867 PB92-116375 PC A04/MF A01 National Inst. of Standards and Technology (EEEL), Boulder, CO. Electromagnetic Technology Div Metrology for Electromagnetic Technology: A Bibliography of NIST Publications.

M. E. DeWeese. Aug 91, 69p NISTIR-3972
Supersedes PB91-132266.

Keywords: \*Metrology, \*Bibliographies, Optical com-munication, Optical fibers, Magnetic measurement, Superconducting devices, Superconductors, Optoe-lectronic devices, Electrooptics, Lasers, Cryoelectron-ics, Electromagnetic metrology, Superconducting materials, \*Electromagnetic metrology, Cryoelectronics.

The bibliography lists the publications of the personnel of the Electromagnetic Technology Division of NIST during the period from January 1970 through publication of the report. A few earlier references that are directly related to the present work of the Division are also included.

Not available NTIS PB92-116516 National Inst. of Standards and Technology (NEL), Boulder, CO. Electromagnetic Technology Div. Voltage Calibration Systems Using Josephson Junction Arrays. Final rept.

C. J. Burroughs, and C. A. Hamilton. 1990, 4p Pub. in IEEE (Institute for Electrical and Electronics Engineers) Transactions on Instrumentation and Measurement 39, n6 p972-975 Dec 90.

Keywords: \*Josephson junctions, \*Standards, \*Calibration, Computerized control systems, Arrays, Uses, Reprints, \*Voltage standards.

The recent development of large arrays of Josephson junctions is allowing an ever increasing number of laboratories to maintain intrinsic Josephson voltage standards at an accuracy near 0.05 ppm. The paper reviews the fundamentals of Josephson voltage standards and how computer control makes these standards simple to use in a variety of applications.

100.869 PB92-117167 Not available NTIS National Inst. of Standards and Technology (EEEL), Gaithersburg, MD. Electricity Div.
Influence of Nonsinusoidal Waveforms on Volt-

meters, Ammeters, and Phase Meters.

N. M. Oldham, and T. L. Nelson. 1991, 6p Pub. in Proceedings of IEEE (Institute for Electrical and Electronics Engineers) Winter Power Meeting, New York City, NY., February 3-7, 1991, p7-12.

Keywords: \*Phase meters, \*Voltmeters, \*Ammeters, Waveforms, Tests, Reprints.

The operating principles of various voltmeters, ammeters, and phase meters are described. The results of tests on these instruments at different levels of distortion indicate that phase meters are subject to large, often unpredictable errors while most voltmeters and ammeters respond to the runs value, independent of waveshape.

100,870 PB92-123082 PC A03/MF A01 National Inst. of Standards and Technology (EEEL), Gaithersburg, MD. Electronics and Electrical Engineering Laboratory. 1991 Strategic Plan. Supporting Technology for U.S. Competitiveness in Electronics. R. M. Powell. Nov 91, 38p NISTIR-4714 See also PB92-112309.

Keywords: \*Electrical measurement, Electronics industry, Optical communication, Semiconductor devices, Microwave equipment, Video equipment, Inteoptical fibers, Strategy, Trends, Facilities, Sensors, Metrology, Electronics and Electrical Engineering Laboratory oratory, Competitiveness, US NIST.

Among U.S. manufacturing industries, the electronics industry is the largest employer (1.94 million) and is a close second in shipments (\$266 billion) to the chemical industry (1990). U.S. competitiveness in many fields of electronics has been declining. Improved competitiveness will require outstanding performance from manufacturers in every step required to put a product into service to a buyer; research and development, manufacturing, marketplace exchange, and after-sales support. All of these steps are highly measurement intensive and have outstripped available measurement support. Improved measurement support is an essential part of any successful strategy for improving U.S. competitiveness. The Electronics and Electrical Engineering Laboratory (EEEL), within the National Institute of Standards and Technology, as part of a continuing study of the electronics industry, is identifying measurement needs in important fields of electronics: semiconductors, superconductors, magnetics, microwaves, lightwaves (optoelectronics), power networks, video, electromagnetic compatibility, and complex-system description and testing. The document describés EEEL's strategic plan for a response in terms of both general strategic directions across all of these fields and specific strategic directions for four fields: semiconductors, microwaves, optical-fiber communications, and video. The plan relates these directions to important goals for improved U.S. competitive-

100,871 PB92-126663

(Order as PB92-126614, PC A06/MF A02) National Inst. of Standards and Technology, Boulder,

Optimization Techniques for Permittivity and Per-

meability Determination.
P. D. Domich, J. Baker-Jarvis, and R. G. Geyer.

Included in Jnl. of Research of the National Institute of Standards and Technology, v96 n5 p565-575 Sep/Oct

Keywords: \*Dielectric properties, \*Permeability, \*Permittivity, Mathematical models, Superhigh frequency, Nonlinear analysis. Microwave frequencies, S matrix, Optimization, Yttrium iron garnets, Barium titanates, Nickel ferrite, Polystyrene, Polymers, Glass.

The paper discusses optimization techniques for the determination of complex permittivity and permeability in transmission lines. The traditional theoretical model using scattering parameters is extended into a mathematical regression model that can be solved with widely accepted numerical techniques. This new model produces accurate primary mode results for the samples tested including nonmagnetic and magnetic materials with high dielectric constants. An extension of the model includes responses due to higher order modes. The general model determines parameters to specify the spectral functional form of complex permittivity and permeability and is capable of small corrections to independent variable data including angular frequency, sample length, sample position, and cutoff wavelength. The method provides reliable determination for both low and high permittivity materials.

## **ENERGY**

#### **Electric Power Transmission**

100.872 PB91-162248 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Electricity Div.
Evaluation of Instrumentation Used to Measure AC

Power System Magnetic Fields. Final rept.

M. Misakian. 1991, 11p Pub. in IEEE (Institute of Electrical and Electronics En-

gineers) Transactions on Power Delivery 6, n1 p1-11

Keywords: \*Power systems, \*Magnetic fields, \*Magnetic measurement, AC systems, Instruments, Exposure meters, Performance, Meetings, Tests, Reprints.

A workshop was organized by the AC Fields Working Group for the purpose of evaluating instrumentation designed for measuring power system magnetic fields. The instruments tested varied from simple single axis survey meters to microcontroller based instruments designed for long term data collection and analysis. The working group designed a series of tests which were used to evaluate each instrument. These included calibration and harmonic response tests, tests of susceptibility to high 60 Hz electric fields and electromagnetic interference and the measurement of fields typical of transmission line, appliance, substation and office/shop environments. Results for each of these tests are presented and discussed. With some minor exceptions, the peformance of all instruments was satisfactory.

100.873 PB91-216770 PC A04/MF A01 National Inst. of Standards and Technology (EEEL),

Gaithersburg, MD. NIST Measurement Services: Calibration Service for Current Transformers.

Special pub. (Final) J. D. Ramboz, and O. Petersons. Jun 91, 62p NIST/ SP-250/36

Also available from Supt. of Docs. as SN003-003-03087-2.

Keywords: \*Current transformers, \*Calibration, Electrical measurement, Electric power distribution, Standards, Uncertainty, US NIST.

A calibration service at the National Institute of Standards and Technology (NIST) for laboratory-quality current transformers is described. The service provides measurements of the current ratio and the phase angle between the secondary and primary currents. In the Report of Calibration or Test, the measured ratio is reported as the product of the marked (nominal) ratio and the ratio correction factor. The measured phase angle is reported directly in milliradians (mrad) and is

#### ENERGY

### **Electric Power Transmission**

positive if the secondary current leads the primary. The range of primary-to-secondary current ratios that can be measured with the equipment at NIST extends from 0.25 A:5 A to 12000 A:5 A. The maximum current at the present time is about 20000 A. Estimates of calibration uncertainties, including their sources, are given and quality control procedures are described. For routine calibrations, uncertainties of + or - 0.01% for the ratio and + or - 0.1 mrad for the phase angle are quoted. However, lower uncertainties—to + or -0.0005% or 5 parts per million (ppm) for ratio and + or 0.005 mrad or 5 microrads for phase angle--are possible under the provisions of Special Tests.

100,874 PB92-112341 PB92-112341 PC A06/MF A02 National Inst. of Standards and Technology (EEEL), Gaithersburg, MD. Electricity Div. Research for Electric Energy Systems: An Annual Report.

Annual rept. 1990.
W. E. Anderson. Jun 91, 105p NISTIR-4691
See also report for 1989, PB90-228032. Sponsored by Department of Energy, Washington, DC. Div. of Electric Energy Systems.

Keywords: \*Surges, \*Power transmission lines, \*Electric fields, \*Dielectrics, Kerr cells, Power lines, Chemical detection, Mathematical models, Graphs(Charts).

The report documents the technical progress in four investigations which make up the project 'Support of Research Projects for Electrical Energy Systems,' funded by the U.S. Department of Energy and performed by the Electricity Division of the National Institute of Standards and Technology (NIST). Specifically these investigations include: (1) Measurements of magnetic fields in support of epidemiological and in vitro studies of biological field effects; (2) development of a technique to measure trace amounts of S2F10 in the presence of SF6 and the development of an improved stochastic analyzer for pulsating phenomena; (3) optical and electrical measurements of negative (3) optical and electrical measurements of negative streamers preceding electric breakdown in liquid die-lectrics; and (4) the development of a reference resistive divider for high voltage impulse measurements. The work discussed in the report is part of an ongoing research activity at NIST.

#### **Fuel Conversion Processes**

100,875 PB91-134940 Not available NTIS National Inst. of Standards and Technology (IMSE), Gaithersburg, MD. Ceramics Div.

Effect of Slag Penetration on the Performance of

Magnesia Chrome Refractories in Slagging Gasifi-

Final rept.
S. M. Wiederhorn, R. F. Krause, J. Sun, and G. V.

Sklizkov. 1987, 8p Sponsored by Department of Energy, Oak Ridge, TN.

Fossil Energy Program.

Pub. in Proceedings of Symposium on Materials for Coal Gasification, Cincinnati, OH., October 10-15, 1987, p121-128.

Keywords: \*Coal gasification, \*Magnesite refractories, \*Refractory materials, \*Creep rupture tests, Slags, Magnesium oxides, Microstructure, Creep rupture strength, Creep properties, Bricks, Fractures(Materials), Reprints.

The purpose of the paper is to present a summary of a study on the morphological changes that occur when refractory bricks are penetrated by slag. The study consisted primarily of a microstructural analysis of specimens from a brick that had been removed from a coal gasifier. Laboratory studies were also conducted on newly manufactured brick to clarify the nature of the reactions that occur in practice. Data suggests a strong correlation between the structural stability of the refractory and the viscosity of the intergranular vit-reous phase that forms as a result of slag penetration. In the course of the paper, the effect of viscosity on grain growth and on the creep and creep rupture be-havior of this material is discussed.

100,876 PB91-158592 PB91-158592 Not available NTIS National Bureau of Standards (IMSE), Gaithersburg, MD. Ceramics Div.

Rapporteur's Summary Materials Development for Coal Gasification.

Final rept.

S. J. Dapkunas. 1987, 3p Pub. in Proceedings of ASM Conference on Materials for Coal Gasification, Cincinnati, OH., October 10-15, 1987, p183-185.

Keywords: \*Coal gasification, \*Corrosion, \*Refractories, Steels, Hydrogen sulfide, Chromium additions, Erosion, Sulfidization, Heat resistant materials, Linings, Aluminum oxide, Ceramics, Slags, Concrete, Reviews, Reprints

The operating conditions found in coal gasification systems have long been recognized as placing severe demands on materials of construction. An assessment of the performance of German wartime synfuels plants specifically cited hydrogen sulfide attack of alloy steels in high pressure Lurgi gasifiers as a problem and noted that 23 percent chromium steels were required for adequate corrosion resistance. The energy crisis of the 1970's raised renewed concern for the behavior of materials in coal gasifiers, and several assessments of the performance of materials, particularly for internal environments of dry ash gasifiers, were conducted. Inplant tests and extensive laboratory testing programs identified sulfidation attack of alloys and, in some applications, erosion to be primary modes of alloy deterioration

## **Fuels**

AD-A242 816/7 PC A03/MF A01 National Inst. of Standards and Technology, Gaithers-Short-Duration Autoignition Temperature Meas-

urements for Hydrocarbon Fuels.
Final rept. May 89-Sep 90.
K. C. Smyth, and N. P. Bryner. Jan 91, 49p AFESC/ESL-TR-90-43,

Keywords: Air, \*Autoignition, Control, Decomposition, Determination, Fuels, Heat, High temperature, Hydrocarbons, Ignition, Measurement, Metals, Mixtures, Nickel, Reliability, Short range(Time), Stainless steel, Surfaces, \*Temperature, Test methods, Titanium, \*Hydrocarbon fuels.

This study develops an experimental method for the reliable determination of auto ignition temperatures under a variety of conditions which involve short duration exposures of controlled fuel/air mixtures on three metal surfaces. Over 1100 auto ignition temperature determinations have been made for the ignition of 15 hydrocarbons on heated nickel, stainless steel, and titanium surfaces for three different fuel/air mixtures. The measured autoignition temperatures generally decrease for the larger hydrocarbons and for richer mixtures, with the C2 hydrocarbons having particularly low values. The highest autoignition temperature are observed for nickel surfaces and the lowest for the stainless steel, with titanium being an intermediate case. Relationships between autoignition, radical-based chemical mechanisms and end-gas autoignition (engine knock) are discussed. Most of the previous autoignition data are unsatisfactory since measurements are typically carried out using ASTM E659 test. This test method attempts to measure the autoignition temperature of hydrocarbons fuels in the gas-phase under experimental conditions where it is more likely that ig-nition temperatures for a complex mixture of the products of fuel decomposition are being determined rather than those of the original fuel.

100.878 PB91-133942 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Chemical Thermodynamics Div. MSW Calorimetry. Final rept.

S. Domalski, K. L. Churney, A. E. Ledford, and M. L. Reilly. 1986, 4p Pub. in Mechanical Engineering, p32-35 Aug 86.

Keywords: \*Colorimeters, \*Calorific value, \*Fuels, \*Garbage, Thermodynamic properties, Solid waste disposal, Heat measurement, Combustion, Sampling, Test facilities, Reprints, \*Municipal wastes, Solid

For many years, it has been the opinion of combustion engineers that one cannot sample a multi-ton quantity of municipal solid waste (MSW) and remove a representative gram-size sample for bomb calorimetric measurement. As a response to this concern, a multikilogram capacity combustion flow calorimeter has been designed, constructed, and placed into operation to assess the credibility of the bomb calorimetric determination using gram-size samples. Calorific values de-rived from both gram-size samples in a bomb calorimeter and multi-kilogram-size samples in a large flow cal-orimeter have been compared and found to be in good agreement. The study has shown that the determination of the calorific value of MSW using gram-size samples is credible provided proper attention is paid to sampling, sample size-reduction, and sample subdivi-

100,879

PB91-134403 Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Chemical Process Metrology Div. Gas Flow Measurement: Calibration Facilities and

Fluid Metering Traceability at the National Bureau of Standards.

Final rept.

G. E. Mattingly. 1987, 24p Pub. in Natural Gas Energy Measurement, p219-242 1987

Keywords: \*Flowmeters, \*Flow measurement, \*Natural gas, Fluid flow, Gas flow, Standards, Test facilities, Calibrating, Accuracy, Reprints, \*Calibration.

As the value of scarce fluid resources increases in today's domestic and international market places and process industries so does the need for improved fluid measurement and for improved traceability to primary standards. Both buyers and sellers of fluid products are increasingly concerned about accurate custody transfer. Designers and operators of industrial processes are increasingly concerned about the precision of their fluid measurement to optimize the performance of their continuous production technologies. To satisfy these expressed needs for improved fluid measurements and traceability in the wide range of fluids and conditions required, is a considerable task. The calibration facilities which flow gas and which are currently in use at the National Bureau of Standards (NBS) are described. The performance characteristics of these facilities are given together with corresponding levels of uncertainties.

100,880

PB91-147025 Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Chemical Engineering Science Div. Experimental Evaluation of Selected Orifice Flowmeter Upstream Installations. Final rept.

Prinal rept.

J. A. Brennan, C. F. Sindt, and M. A. Lewis. 1990, 9p. Sponsored by Gas Research Inst., Chicago, IL. Pub. in Proceedings of American Gas Association Distribution/Transmission Conference, Los Angeles, CA., May 7-9, 1990, p594-602.

Keywords: \*Orifice meters, \*Gas meters, \*Standards, Roughness, Flowmeters, Orifices, Specifications, Flow measurement, Gas flow, Pipes(Tubes), Gas pipes, Re-

There are two standards for orifice flow measurement that are the primary references used in the gas industries around the world. These standards differ significantly on some installation specifications. The differences can profoundly affect the design, cost, and measurement accuracy of meter stations. Revisions to the standards are currently being completed. A new flow equation has been developed, and serious consideration given to changing some of the installation specifications. New experimental test results are the basis for changing the installation specifications on pipe roughness and flow conditioner location. These two parameters are being studied both individually and collectively. Results from tests on orifice flowmeters ranging from 3 to 24 in are presented.

100.881

PB91-148791 Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Chemical Engineering Science Div. Effect of Tube Bundle Flow Conditioners on Orifice Meter Discharge Coefficients.

Final rept K. M. Kothari, J. A. Brennan, and J. Gorter. 1990, 9p

Sponsored by Gas Research Inst., Chicago, IL. Pub. in Proceedings of International Gas Research Conference, Tokyo, Japan, November 6-9, 1989, p541-549 1990.

Keywords: \*Flow regulators, \*Flow measurement, Flowmeters, Natural gas, Nitrogen, Tubes, Reynolds number, Reprints, \*Tube discharge flow conditioners, Discharge coefficients.

Two experimental test programs on the use of tube bundle flow conditioners upstream of an orifice flowmeter have been completed. One program used a flange tapped 100 mm orifice flowmeter in nitrogen gas at pressures of approximately 4 MPa and the other used a 600 mm orifice flowmeter in natural gas at pressures of approximately 6 MPa. The 100 mm flowmeter tests were run at a Reynolds number near 1,000,000 and the 600 mm flowmeter test covered the Reynolds number range of 1,000,000 to 55,000,000 and included D-D/2, flange, and corner tappings. Both programs included several beta ratio orifice plates. Test results clearly show that placement of the flow conditioner 7 pipe diameters upstream of the orifice plate can cause bias measurement errors compared to long pipe data. For some beta ratios, these bias errors exceeded 1%.

100 882

PB91-162214 Not available NTIS National Bureau of Standards (NEL), Boulder, CO. Thermophysics Div.

Speed of Sound of Natural Gas Mixtures.

Final rept.

Plus rept.

R. D. McCarty. 1986, 7p

Pub. in Proceedings of International Symposium on Fluid Flow Measurement, Arlington, VA., November 16-19, 1986, 7p.

Keywords: \*Natural gas, \*Acoustic velocity, Equations of state, Mathematical prediction, State of the art, Mixtures, Density, Reprints.

Accurate values for the speed of sound in natural gas mixtures are important in the application of sonic metering devices and in many design applications. In the case of mixtures, it is not possible to obtain experimentally determined speed of sound data for all possible compositions of the pure components found in natural gases. The alternative is a mathematical model of acceptable accuracy which allows the prediction of the speed of sound at an arbitrary state point composition. The paper describes the 'state of the art' for the prediction of the speed of sound for natural gases.

100,883 PB91-162271 Not available NTIS National Inst. of Standards and Technology (MSEL),

Gaithersburg, MD. Polymers Div.
Bioprocessing of Fossil Fuels Using Hyperthermophilic Archaebacteria.
Final rept.

G. J. Olson, T. L. Peeples, I. I. Blumentals, R. N. Schicho, and S. H. Brown. 1989, 16p Pub. in Proceedings of Symposium on Biological Proc-

essing of Coal and Coal-Derived Substances, Palo Alto, CA., May 15-19, 1989, p2-53-2-68.

Keywords: \*Coal, \*Metabolism, \*Sulfur, \*Desulfurization, Bacteria, Thermophiles, Hydrogen sulfide, Cystine, Thiols, Sulfides, Reprints, \*Pyrococcus furiosus, Bioprocessing.

Studies on the metabolism of sulfur in model compounds and in coals at 98-100 C were conducted using the hyperthermophilic archaebacterium, Pyrococcus furiosus (P. furiosus). The bacterium produced hydro-gen sulfide from elemental sulfur, cystine, methyl tri-sulfide and thiocystine. In addition, mercaptans were detected when the organism was grown in the presence of disulfides. Instability of several of the model compounds at the high incubation temperatures may have accounted for some of the observed transformations. P. furiosus produced small amounts of hydrogen sulfide when grown in the presence of coals given oxidative or perchloroethylene treatments. A continuous feed process at 98 C was demonstrated with refuse coal containing over 1% by weight elemental sulfur. At a dilution rate of 0.25 per hour, coal sulfur decreased from 6.4 to 5.2%.

100,884 PB91-175299

Not available NTIS

National Bureau of Standards (NEL), Gaithersburg, MD. Applied and Computational Mathematics Div. Gas Analysis Modeling System.

Final rept. R. P. O'Neill, W. G. Kurator, B. Mariner-Volpe, W. A. Trapmann, and J. Heinkel. 1984, 19p Pub. in Analytic Techniques for Energy Planning, p265-

Keywords: \*Natural gas, \*Gas pipelines, \*Gas supply, \*Energy models, Gas distribution, Reserves, Fuel consumption, Regulations, Mathematical models, Reprints, \*Gas Analysis Modeling System.

The Gas Analysis Modeling System (GAMS) has been developed to provide EIA with the ability to study issues associated with natural gas supply and pipeline regulatory options. GAMS represents aggregates of the major United States pipelines, domestic supply sources and end uses as well as the corresponding regulations.

100.885

PB91-195339 Not available NTIS National Bureau of Standards (IMSE), Gaithersburg, MD. Polymers Div.

Recent Progress in Coal Bioprocessing Research in the United States: Scope and Areas Needing Further Research. Final rept.

G. J. Olson. 1988, 7p

Pub. in Conservation and Recycling 1, n3-4 p319-325 Aug 88.

Keywords: \*Coal preparation, Desulfurization, Microorganisms, Research management, Solubility, Reprints.

The paper summarizes the scope of recent coal bio-processing research in the United States including de-sulfurization, solubilization, and other aspects of coal cleaning. Measurement and standards needs are discussed, areas of controversy or neglect which require additional research are also described.

100.886

PB91-203323 Not available NTIS National Inst. of Standards and Technology (IMSE), Gaithersburg, MD. Polymers Div. Biological Sulfur Oxidation and Reduction for Coal

Sulfur Speciation and Desulfurization. Final rept

R. M. Kelly, R. N. Schicho, S. H. Brown, J. P. Soisson, I. I. Blumentals, G. J. Olson, and E. J.

Parks, 1989, 15p Pub. in Proceedings of the Annual EPRI (Electric Power Research Institute) Conference (13th) on Fuel Science and Conversion, Santa Clara, CA., May 18-19, 1988, p7-3-7-17 1989.

Keywords: \*Qualitative analysis, \*Sulfur ions, \*Coal, \*Desulfurization, \*Bioassay, Biochemistry, Oxidation, Reduction(Chemistry), Bacteria, Thiobacillus oxidans, Carbon sulfides, Microbiology, Reprints, Pyrococcus furiosus, Pyrodictium brockii, Speciation.

Sulfur speciation in coal is limited by uncertainties in the analytical methods used. Assays based on biological activity may eliminate some of these limitations. bacteria capable of elemental sulfur oxidation(Thiobacillus thiooxidans) or elemental sulfur reduction (Pyrococcus furiosus and Pyrodictium brockii), it was possible to determine the approximate levels of the sulfur species in four different coal samples. It was found that in three of the coal samples (Illinois No. 6, Indiana No. 5, and an Australian coal), only trace amounts of elemental sulfur could be detected by bioassay. However, an Indiana bog coal was found to have in excess of 1% (by weight) elemental sulfur content. Existing analytical methodology for coal sulfur speciation was shown to characterize the sulfur fraction as organic. In all cases, the results obtained by bioassay were reinforced through chemical analysis following CS2 extraction of the coals. Elemental sulfur levels in the Indiana bog coal could be determined by either oxidative or reductive microbial processing. The results obtained here suggest that bioassay can be used to screen coals for elemental sulfur content and may provide an alternate and complementary probe for sulfur speciation.

100,887 PB92-108927 PC A03/MF A01 National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Center for Fire Research.

Short-Duration Autoignition Temperature Measurements for Hydrocarbon Fuels. K. C. Smyth, and N. P. Bryner. Dec 90, 48p NISTIR-

4469 Contract JON-2104-3039

See also AD-778 998. Sponsored by Air Force Engineering and Services Center, Tyndall AFB, FL.

Keywords: \*Autoignition, \*Hydrocarbons, \*Fuels, Temperature measurement, Tests, Laboratory equip-

The autoignition of hydrocarbon fuels on hot surfaces is a process of practical significance which occurs when self-sustained combustion of a gas mixture is initiated. Possible prevention can be accomplished by choosing fuels of the proper molecular structure, by choosing the composition, coatings, or treatment of the hot surface, or by other intervention strategies. The goal of the present investigation is to devise a reliable method for measuring the autoignition behavior of hydrocarbon fuels in order to formulate appropriate strategies to reduce autoignition tendencies.

## **Heating & Cooling Systems**

100,888

PB91-134221 Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Building Physics Div.

Method for Measuring Heat Loss from Under-

ground Heat Distribution Systems.

inal rept.

T. Kusuda, J. B. Fang, and W. M. Ellis. 1987, 17p Pub. in Thermal Insulation: Materials and Systems, ASTM STP 922, p52-68 1987.

Keywords: \*Heat loss, \*Heat measurement, \*Thermal measurements, Pipes(Tubes), Distribution systems, Heat transmission, Field tests, Heat transfer, Model tests, Reprints, \*Heat distribution systems.

A simple procedure to obtain the in situ determination of heat loss from an underground heat distribution system is described. The proposed procedure for estimating the heat loss from underground heat distribution systems consists of making a series of temperature and thermal conductivity measurements on the ground grid in the vicinity of the pipe system and de-ducing the heat loss by statistically determining the parameters of a mathematical model using the gathered data. Verification of the procedure was tested in a simulated scale model of an underground system using an insulated sandbox. The scale model is a two-pipe system buried 0.3045 m(12 in.) below the top surface of a 0.66-m(26-in.)-wide, 0.71-m(28-in.)-high, and 1.22-m(48-in.)-long sandbox. The test pipes are two electrically heated steel pipes having an outside diameter of 3.37 cm(1.325 in.). The walls of the sandbox are insulated by 5.08-cm(2-in.)thick expanded polystyrene board. The heat loss measurements from this simulated underground heat distribution system were tained for pipe surface temperatures of 66 C (150.9 F), 93.8 C (200.8 F), and 149.2 C (300.7 F) for three different sand moisture contents (dry, 10%, and 13%). Relatively good agreement was obtained-between the measured electrical power input to the test pipes and the system heat loss estimated by the sand temperature profile around the pipes and sand thermal conductivity measured by the thermal needle technique.

100.889

PC A05/MF A01 PB91-144386 National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Center for Building Technology.

Computer Program for Simulation of HVAC/Lighting Interactions: Initial Report. G. N. Walton. Dec 90, 99p NISTIR-4472

Sponsored by Department of Energy, Washington, DC., and Electric Power Research Inst., Palo Alto, CA.

Keywords: \*HVAC systems, \*Lighting systems, \*Computerized simulation, \*Buildings, Algorithms, Interactions, Thermal measurements, Energy audits, HLITE computer program, National Institute of Standards and Technology.

The report describes the initial release of the HLITE program, which simulates the thermal interaction of lighting and HVAC systems. The program was developed to extend the results of an experimental study in

#### **ENERGY**

## **Heating & Cooling Systems**

HVAC/lighting interaction being conducted at the National Institute of Standards and Technology (NIST). It will serve in planning future experimental test cases and in the development of algorithms that can be incorporated into larger building energy analysis programs. The interim report covers the first phase of the development of HLITE which simulates the NIST HVAC/lighting test facility. Future planned developments will expand its capabilities to larger facilities with more complete thermal interactions. The computer program is based on a simple combined explicit and implicit time integration scheme for a finite volume model which may be applicable to a much broader range of building simulations.

PB91-144410 PC A03/MF A01 National Inst. of Standards and Technology (NML), Boulder, CO. Chemical Engineering Science Div. Effect of Noble Gas Mixtures on the Performance of Regenerative-Type Cryocoolers Analytical Esti-

D. E. Daney. Sep 90, 38p NISTIR-90/3936 Sponsored by Air Force Space Technology Center, Kirtland AFB, NM.

Keywords: \*Regenerative cooling, \*Helium, \*Krypton, \*Argon, \*Binary mixtures, \*Heat transfer, Cryogenics, Prandtl number, Viscosity, Thermal conductivity, Performance evaluation, Graphs(Charts).

The authors compare the performance of regenerators that use noble gas mixtures to the performance of those that use pure helium gas. Both helium-argon and helium-krypton mixtures are investigated. For some heat transfer surfaces, a modest gain in heat transfer can be achieved with these mixtures. The concomitant increase in pressure drop, however, more than offsets the heat transfer gain so the net regenerator loss increases for all cases they evaluated. The dependence of heat transfer on Prandtl number (Pr) has not been measured for the range associated with noble gas mixtures, 0.2 < Pr < 0.5, and they estimate that the uncertainty from the source can exceed 20 percent. The authors give the estimates for the transport properties (Prandtl number, viscosity, and thermal conductivity) of helium-argon and helium-krypton mixtures because of the absence of experimental data at low temperature.

100,891 PB91-174516 Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Building Environment Div.

Research and Development of Heat Pumps Using Nonazeotropic Mixture Refrigerants. Final rept.

J. M. Calm, and D. A. Didion. 1985, 8p

Sponsored by Electric Power Research Inst., Palo Alto, CA.

Pub. in ASHRAE (American Society of Heating, Refrigerating and Air-Conditioning Engineers) Technical Data Bulletin, v1 n9 p132-139 Jun 85.

Keywords: \*Refrigerants, \*Heat pumps, Air conditioning equipment, Cooling systems, Air conditioners, Research projects, Thermodynamic properties, Coolants, Heating systems, Working fluids, Reprints, \*Nonazeotropic mixtures.

Although nearly a century has passed since the use of multicomponent refrigerants was first proposed, such refrigerants have achieved only extremely limited application. Further research and development will be needed before widespread use of nonazeotropic mixture refrigerants will be commercially attractive. The paper summarizes a workshop conducted to identify these research and development needs.

100,892 PB91-206706 PC A04/MF A01 National Inst. of Standards and Technology (BFRL), Gaithersburg, MD.

Measurement and Evaluation of Lighting/HVAC

S. J. Treado, and J. W. Bean. May 91, 55p NISTIR-4429

Keywords: \*Lighting systems, \*HVAC systems, \*Cooling load, \*Energy consumption, Temperature measurement, Energy conservation, Heat transfer, Heat transmission, Walls, Ventilation, Test facilities.

The interaction of building lighting and HVAC systems and the effects on cooling load and lighting system performance are being evaluated using a full-scale test facility at the National Institute of Standards and Technology (NIST). The test facility and measurement methodology are described, along with sample test data and performance evaluation results. The implications of measurement uncertainty on results are dis-

100 893 PB92-126432 PC A07/MF A02 National Inst. of Standards and Technology, Gaithers-

Evaporator Performance Investigation for Residential Air-Conditioning Application Using Mixed Refrigerants.

M. Chwalowski. Nov 91, 148p NISTIR-4723 See also PB87-152286. Sponsored by Electric Power Research Inst., Palo Alto, CA. Nuclear Power Div.

Keywords: \*Evaporators, \*Air conditioning, \*Reliability, Residential buildings, Heat exchangers, Refrigerants, Mixtures, Performance evaluation, Design criteria, Effectiveness, Profiles, Nonazeotropic.

The design of the heat exchanger utilizing nonazeotropic refrigerant in an air conditioning application pre-sents unique problems due to the phase change of the moist air and the variable specific heat of the evaporat-ing refrigerant mixture. The study discusses the per-formance analysis and the design procedure of a cross counterflow heat exchanger working as an evaporator in an experimental system which simulated a residential air conditioning application. The effect of the change of the mixture composition on heat exchanger performance was evaluated. The focus of the theoreti-cal study was the development of the effectiveness/ Number of Transfer Units (NTU) (Exit/NTU) relationships with the use of the experimentally derived quanti-ties for moist air flowing across the heat exchanger.

PB92-126440 PC A04/MF A01 National Inst. of Standards and Technology, Gaithers-PC A04/MF A01 burg, MD.

Testing and Rating of an Atmospheric, Gas-Fired Furnace Equipped with a Burner Air Inlet Damper. S. T. Liu, G. E. Kelly, and C. P. Terlizzi. Nov 91, 61p NISTIR-4717

See also PB-289 484. Sponsored by Department of Energy, Washington, DC. Office of Conservation and Renewable Energy.

Keywords: \*Gas furnaces, Air flow, Heat exchanger, Draft control systems, Energy consumption, Tracer techniques, Tests, Flue gases, Gas burners, \*Burner box inlet dampers, Atmospheric gas furnaces, Flue dampers, Draft diverters.

An atmospheric furnace with an integral draft diverter and an electro-mechanical burner box inlet damper was tested by the tracer gas method for the development of a test procedure. Tracer gas tests were conducted under two conditions: with the diverter open, and with the diverter sealed and the stack restricted. Test results indicated that the flue gas flow patterns inside the heat exchanger were different for the two conditions. There was reverse flow in one of the clam shells when the diverter was open, but no flow reversal when the diverter was sealed. The off-cycle sensible loss which was a measure of the effectiveness of the burner box inlet damper gave similar value for both conditions. Because of the change in flow pattern and the fact that the furnace normally operated in the field with the diverter open, a recommended test procedure was developed which requires that the tracer gas test should be conducted with the diverter open. A calculation procedure was developed to compute the annual fuel utilization efficiency for the type of furnaces that employ a burner box inlet damper or flue damper for off-cycle loss reduction.

## Policies, Regulations & Studies

100,895 PB91-147728 Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Office of Energy-Related Inventions.
Feasibility of Using Knowledge-Based Systems for Aiding Inventors. Final rept.

J. L. Merchant. 1986, 14p Pub. in Proceedings of the Annual Meeting of the Technology Transfer Society (11th), Indianapolis, IN., June 23-26, 1986, p1-12. Keywords: \*Research management, \*Expert systems, Research projects, Knowledge bases(Artificial intelli-gence), Inventions, Computers, Computer systems programs, Computer applications, Reprints, \*ERIP(Energy-Related Inventions Program), Department of Energy.

The Energy-Related Inventions Program (ERIP) is a small program whose purpose is to provide support to independent inventors and small businesses with promising energy-related inventions and to move these inventions closer to the marketplace. The National Bureau of Standards (NBS) provides, at no cost to the inventor, evaluations of energy-related inventions and recommends those it considers promising to the Department of Energy (DOE). In turn, DOE pro-vides financial support and/or help in marketing an invides financial support and/or help in marketing an inventor's idea. The objective of the task is to estimate the potential for use of computers to assist inventors in the development of their ideas or to provide synergism for the development of new ideas. The paper will explore the current state of knowledge-based systems and other computer software as they could relate to invention, and recommend ERIP actions that would lead to realization of their potential.

100.896

PB91-158659 Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Office of Energy-Related Inventions. Evaluation of Building Systems Inventions.

Final rept.

Pub. in Proceedings of Conference on Energy: An Integrated Approach, Chattanooga, TN., April 30-May 2, 1986, p97-100.

Keywords: \*Grants, \*Inventions, \*Buildings, Meetings, Energy conservation, Research management, US NBS, US DOE, Reprints.

One part of the United States Federal Nonnuclear Energy Research and Development Act of 1974 di-rects the National Bureau of Standards (NBS) to evaluate all promising nonnuclear energy-related inventions for the purpose of obtaining direct grants for their development from the Department of Energy (DOE). The program provides an opportunity for independent inventors and small businesses to obtain Federal assistance in developing and commercializing their inventions.

100,897 PB91-167288 PC A03/MF A01 National Inst. of Standards and Technology (CAML),

Gaithersburg, MD.

DISCOUNT-A Program for Discounting Computations in Life-Cycle Cost Analyses. User's Guide
and Reference Manual. Final rept.

S. R. Petersen. Jan 91, 22p NISTIR-4513 Prepared in cooperation with Federal Energy Management Program, Washington, DC.

Keywords: \*Energy conservation, \*Energy sources, \*Life cycle costs, \*Cost analysis, Economic analysis, Projects, Buildings, Value, Discounted cash flow, Interest rate, Present worth, Return on investment, User manuals(Computer programs), DISCOUNT computer program.

The DISCOUNT computer program has been prepared as an aid to implementing life-cycle cost evaluations of potential energy conservation and renewable energy projects in new and existing Federal buildings. It can also be used for evaluating similar projects in the private sector and at the state and local government levels. The DISCOUNT program computes discount factors and related present values, future values, and periodic payment values of cash flows occurring at known points in time. DISCOUNT computations are especially useful in life-cycle cost analysis, financial analysis, and engineering-economics problems not requiring comprehensive summation and reporting. DIS-COUNT performs all of the functions of standard discounting tables, computing present values of future counting tables, computing present values of future amounts, future values of persent amounts, present and future values of periodic payments, and periodic payments corresponding to present and future amounts. In addition, DISCOUNT computes the present value of periodic payments which increase at known rates over time, and the present value of energy costs which increase at rates projected by the U.S. Department of Energy for use in Federal life-cycle cost analyses. DISCOUNT provides the added flexibil-

## Policies, Regulations & Studies

ity of accepting non-integer discount rates, time periods, and escalation rates in its computations. DIS-COUNT runs on most IBM PC and compatible microcomputers with no special equipment requirements.

PB91-507970 CP D02 National Inst. of Standards and Technology (CAML), Gaithersburg, MD. Office of Applied Economics.
Building Life Cycle Cost Computer Program, Version 3.2 (for Microcomputers).

Jul 91, 2 diskettes NIST/SW/DK-91/013 Supersedes PB90-501206 and PB90-501198. The software is on two 360K, 5 1/4 inch diskettes, double density. Documentation included; may be ordered separately as PB91-159764.

Keywords: \*Software, \*Buildings, \*Life cycle costs, \*Economic analysis, Operating costs, Benefit cost analysis, Energy conservation, Savings, Return on investment, Cash flow, Project management, Diskettes, Savings-to-investment ratio.

Building Life Cycle Cost (BLCC) Computer Program 3.0 is an economic analysis software package for evaluating investments in buildings and building systems which reduce their long-term operating costs. It is especially useful for evaluating the costs and savings of energy conservation projects in buildings. BLCC computes life-cycle costs, savings-to-investment ratio, net savings, internal rate of return, and cash flow analysis for project alternatives. It is appropriate for Federal and private sector use, as well as for state and local governments. BLCC runs on most IBM-PC and compatible microcomputers, with or without a hard disk. No special computer hardware or graphics capabilities are needed.

100,899 PB92-112515 PC A04/MF A01 National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Center for Computing and Applied Mathematics.

Mathematics.

Energy Prices and Discount Factors for Life-Cycle
Cost Analysis 1992. Annual Supplement to NIST
Handbook 135 and NBS Special Publication 709.
B. C. Lippiatt. Oct 91, 63p NISTIR-85/3273-6
See also report for 1991, PB91-113613. Sponsored by
Department of Energy, Washington, DC. Federal
Energy Management Program Staff.

Keywords: \*Cost analysis, \*Prices, \*Life cycle costs, Fuels, Residential buildings, National government, Electric appliances, Economic analysis, Energy conservation, Energy supplies, Tables(Data), \*Federal Energy Management Program.

The report is the 1992 annual edition of energy prices and discount factors for performing life-cycle cost analyses of energy conservation and renewable energy projects. It supports the Federal life-cycle costing methodology by updating the energy price projections and descount factors that are described, explained, and illustrated in NIST Handbook 135 (HB piairied, and illustrated in NIST Handbook 135 (HB 135). It supports private-sector life-cycle cost analysis by updating the energy price indices that are described, explained, and illustrated in NBS Special Publication 709 (SP 709). It also supports the Energy Conservation Mandatory Performance Standards for New Federal Residential Buildings (10 CFR 435) by providing a table of factors for updating appliance label values.

#### Reserves

100.900 N91-20219/2

(Order as N91-20207/7, PC A05/MF A01) National Bureau of Standards (IMSE), Gaithersburg,

Kelvin Water-Drop Experiment.

R. D. Shull. Jan 90, 3p In NASA, Langley Research Center, National Educa-tors' Workshop: Update 1988. Standard Experiments in Engineering Materials Science and Technology p

Keywords: \*Electric potential, Experimentation, \*Procedures, \*Water, Copper, Electrons, Metal plates, Students.

This experiment was originally designed and per-formed by Lord Kelvin (William Thomson) in the late 1800's to demonstrate the creation of an electric potential simply by means of dividing up a body of flowing water. The objective is to demonstrate the power of electrical forces in a material as common as water and to help teach the student that even simple, well understood phenomena sometimes present unexpected re-sults that, at first thought, defeat explanation. The ex-perimental equipment and procedure are explained.

#### Solar Energy

100,901 PB91-159152 Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Building Equipment Div.

Method for Characterizing the Thermal Performance of a Solar Storage Wall from Measured Data. Final rept.

Final rept.
J. Seem, and E. Hancock. 1985, 12p
Sponsored by Department of Energy, Washington, DC.
Passive and Hybrid Solar Energy Div.
Pub. in Proceedings of ASHRAE/DOE/BTECC Conference on Thermal Performance of the Exterior Envelopes of Buildings III, Clearwater Beach, FL., December 2-5, 1985, p1304-1315.

Keywords: \*Heat transfer, \*Thermal energy storage systems, \*Solar energy, \*Walls, Regression analysis, Least squares method, Calorimeters, Heat flux, Solar architecture, Heat transmission, Construction materials, Reprints.

A technique is presented for characterizing the dynamic performance of a thermal-storage wall based on the data obtained from a series of temperature and heat flux measurements. It is shown that the coefficients of a transfer function model can be estimated directly from data using linear least squares regression. Data from the National Bureau of Standards (NBS) Passive Solar Component Calorimeter are used to demonstrate that the technique can be successfully applied. The transfer function techniques are potentially applicable to linear systems with time-invariant properties. It is also shown that a very simple set of parameters can be derived from the transfer function coefficients to characterize the steady-state performance. Only one parameter for each system input is required to pre-dict long-term average thermal performance of the component.

## General

PR91-178871 PC A09/MF A01 National Inst. of Standards and Technology, Gaithersburg, MD. Office of Energy-Related Inventions Energy Related Inventions Program: A Joint Pro-gram of the Department of Energy and the Nation-al Institute of Standards and Technology. Status Report for Recommendations 1 through 250. Mar 91, 179p NISTIR-4533 Supersedes PB90-225988.

Keywords: \*Inventions, \*US NIST, \*US DOE, Recommendations, Indexes(Documentation).

A brief description of the Energy-Related Inventions Program and all inventions recommended by the National Institute of Standards and Technology to the De-partment of Energy since the inception of the program, including a brief summary of the current status of each.

100,903 PB91-184770 PC A13/MF A02 PB91-184770 PC A13/MF A02
National Inst. of Standards and Technology, Gaithersburg, MD. Office of Energy-Related Inventions.
Energy Related Inventions Program. A Joint Program of the Department of Energy and the National Institute of Standards and Technology. Status Report for Recommendations 251 through 523.

Mar 91 - 2980 NISTIR 4524 Mar 91, 298p NISTIR-4534 Supersedes PB90-221813.

Keywords: \*Inventions, Technology innovation, Product development, Recommendations, Evaluation, Grants, US DOE, \*Energy related inventions program,

The Energy-Related Inventions Program was established in 1975. Since its inception over 27,000 inventions have been evaluated. As of the printing of the report, 523 have been recommended to the Department of Energy. The report supercedes NISTIR 4313 and summarizes the status of Inventions 251 through 523. A companion report (NISTIR 4533) summarizes recommended inventions 1 through 250.

# ENVIRONMENTAL **POLLUTION &** CONTROL

#### Air Pollution & Control

100.904

Not available NTIS PB91-158741 National Bureau of Standards (NML), Gaithersburg, MD. Chemical Thermodynamics Div.

Thermodynamic Data for Modeling of Flue Gas

Cleanup Systems (Abstract for Poster Session). Interim rept. Sep 86-Jun 87. D. Garvin, M. W. Chase, and S. Abramowitz. 1987,

Contract DE-Al22-83PC60425

Sponsored by Department of Energy, Pittsburgh, PA. Pittsburgh Energy Technology Center. Pub. in Proceedings of Coal Utilization and Environmental Control Contractors' Review Meeting, Gaithers William 1987 (2018) ersburg, MD., July 7-9, 1987, 3p.

Keywords: \*Sulfur dioxide, \*Nitrogen oxides, \*Flue gases, Thermochemistry, Air pollution control, Stationary sources, Abstracts, Data, Reprints.

A thermodynamic data system has been designed for use with flue gas control systems. Values of thermodynamic properties have been selected for the major species in SOx-NOx systems. For each selected value a reliability is given together with documentation of the source of the value. Data are given for chemical processes in the gas, solid and solution phases. Both tabular and graphical presentations are used. A new analysis has been made of the solubility of SO2 and its ionization in aqueous solution.

100,905

PB91-167353 PC A03/MF A01 National Inst. of Standards and Technology (BFRL),

Gaithersburg, MD.
Proposed Standard Practice for Assessing the
Performance of Gas-Phase Air Cleaning Equipment.

S. Silberstein. Mar 91, 23p NISTIR-4523

Keywords: \*Indoor air pollution, \*Air cleaners, \*Air pollution control equipment, \*Standards, Air flow, Activated carbon, Service life, Air filters, Performance, Contaminants, Airborne wastes.

The proposed standard practice provides a general and flexible laboratory method for assessing the per-formance of equipment for controlling indoor concen-trations of gas-phase air contaminants. Using a canister filled with adsorption media, a profile of break-through concentration over time is obtained during each test conducted at a fixed contaminant challenge concentration. Results of tests performed for different contaminants and different challenge concentrations can be used for estimating the useful life of air cleaning equipment, and for comparing equipment. The information will be useful to the engineer for the design and selection of such equipment. selection of such equipment.

100.906

PB91-175539 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Molecular Spectroscopy Div.

#### **ENVIRONMENTAL POLLUTION & CONTROL**

#### Air Pollution & Control

Infrared Spectroscopy Applied to Atmospheric Chemistry. Final rept.

A. G. Maki. 1985, 7p

Pub. in Proceedings of CMA/NBS Workshop on Atmospheric Spectra, Gaithersburg, MD., November 3-4, 1983, p1-7 1985.

Keywords: \*Atmospheric composition, \*Infrared spectroscopy, Absorption spectra, Trace amounts, High resolution, Monitoring, Detection, Reprints.

The requirements of laboratory infrared spectroscopy for applications to detection and monitoring of molecular species present in trace amounts in the earth's atmosphere are reviewed. A critical evaluation is presented of the problems encountered in accurate determination of the frequencies, intensities, and line shapes of the absorption features. Problems encountered with transient, unstable species and the effect of perturbations on the intensities are discussed.

100.907 PB91-187146 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Building Environment Div.

Multi-Zone Dispersal Analysis by Element Assem-

Final rept.

J. W. Axley. 198**9**, 18p Sponsored by Department of Energy, Washington, DC., Environmental Protection Agency, Washington, DC., and Consumer Product Safety Commission, Washington, DC.

Pub. in Building and Environment 24, n2 p113-130

Keywords: \*Indoor air quality, \*Transport properties, \*Flow models, Particulates, Mass flow, Air pollution, Mathematical models, Computerized simulation, Buildings, Air flow, Reprints.

An element-assembly formulation of multi-zone contaminant dispersal theory that is not limited to the well-mixed zone idealization is described. In the approach flow systems are idealized as assemblages of elements that model specific instances on contaminant mass transport within a system. A general form and specific examples of element equations are presented. The process of assembling the element equations to form system equations and the qualitative character of the resulting system equations is discussed. Solutions options are outlined, examples of application are presented, and one implementation of the theory, the CONTAM family of programs developed at NBS, is briefly described.

100.908 Not available NTIS PB91-195347 National Bureau of Standards (NML), Gaithersburg, MD. Inorganic Analytical Research Div. Development of a New Tracer Technology Using Enriched Rare-Earth Isotopes. Final rept.

J. M. Ondov, and W. R. Kelly. 1988, 1p Pub. in Abstracts of Papers of the American Chemical Society 195, p84 Jun 88.

Keywords: \*Isotopic labeling, \*Rare earth elements, \*Fly ash, \*Flue gases, \*Electric power plants, \*Neodymium 148, Technology assessment, Field test, Coal combustion, Design, Stationary sources, Deposition, Tracer techniques, Reprints.

Under funding from the Electric Power Research Institute, the authors are developing a new particulate tracer technology suitable for use in power plant studies using enriched rare-earth (RE) isotopes and advanced tracer delivery techniques. Highly enriched RE isotopes are nontoxic, chemically and radiologically stable, and are available at modest cost. The relative abundances of most RE isotopes are invariant in nature and can be measured with great precision by thermal ionization mass spectrometry. Since there are no industrial sources of enriched RE isotopes, they can be used as definitive tracers. Design calculations suggest that signal-to-noise (S:N) ratios > 500:1 could be achieved in ambient aerosols 100-km downwind of a 425-MW(e) power plant with a release rate of only 126 mg (148)Nd/hr. Error analyses suggest that the technique offers a >40,000-fold advantage over previously proposed whole-element tracer schemes. Results of limited field tests suggest that S:N ratios adequate for detection at 100 km could be achieved in ambient aerosol particles less than or equal to 10 micrometers from a 100 MW(e) coalfired power plant

with a release rate as little as 13 mg/hr. The S:N ratios of submicrometer particles are enormous and should permit detection over 1000-km distances. The tests further suggest that fly ash particles can be effectively 'tagged' by coagulation with fine residue particles made with simple two-fluid atomizers operated at elevated pressure.

100 909 Not available NTIS PB91-195420 National Bureau of Standards (NEL), Gaithersburg, MD. Building Environment Div.

Air Exchange and Pollutant Concentration Measurements in Two Office Buildings.

A. Persily, W. S. Dols, and R. Grot. 1988, 10p Sponsored by Geological Survey, Reston, VA., and General Services Administration, Washington, DC. Pub. in Proceedings of CIB Conference Health Buildings '88, Stockholm, Sweden, September 1988, p591-

Keywords: \*Air pollution monitoring, \*Commercial buildings, \*Carbon monoxide, \*Carbon dioxide, \*Formaldehyde, \*Radon, \*Indoor air pollution, \*Air circulation, Air quality, Air flow, Ventilation, Volatile organic compounds, Garages, Tracer techniques, Office buildings, Reprints, Tracer gas analysis.

Long term measurements of air exchange rates and indoor pollutant concentrations were made in two, mechanically ventilated office buildings. The measurements employed automatic tracer gas measurement systems for the continuous monitoring of air exchange rates. Automated measurements of carbon monoxide and dioxide were made concurrently. Passive monitors were employed to measure concentrations of radon and formaldehyde. Measurements were also made of particulate concentrations and for the identification of volatile organic compounds. The first building had a history of indoor air quality and thermal comfort complaints, but the air exchange rates were very high and no excessive pollutant levels were identified. Problems of intake air quality did occur periodically. The second building is recently constructed and has had few indoor air quality problems. Airflow from the under-ground parking garage into the office space has led to elevated carbon monoxide levels at times.

100,910

PC A07/MF A01 PB91-206722 National Inst. of Standards and Technology (BFRL), Gaithersburg, MD.

User Manual NBSAVIS CONTAM88. A User Interface for Air Movement and Contaminant Dispersal Analysis in Multizone Buildings.

Analysis in Multizone buildings.

R. A. Grot. Jun 91, 150p NISTIR-4585

Sponsored by Department of Energy, Washington, DC.

Building Services Div., Consumer Product Safety Comission, Washington, DC. Directorate of Engineering Science, and Environmental Protection Agency, Research Triangle Park, NC. Atmospheric Research and Exposure Assessment Lab.

Keywords: \*User manuals(Computer programs), \*Indoor air quality, \*Air flow, Buildings, Indoor air pollution, Ventilation, Steady state, Air quality, Contaminants, Leakage, Environmental quality, CONTAM88 computer program.

The manual describes the usage of three computer programs for analyzing the air movement and indoor air quality in multizone buildings. The first program NBSAVIS creates and edits a building description and generates the leakage, fan and contaminant data necessary to predict the air infiltration and internal air movement in a building and perform an indoor air quality analysis. These data are used by the program CONTAM88 which calculates the air flows and both dynamic and steady state levels of indoor contaminants. CONTAMEZ also produces an output file which can serve as the input for the NIST programs CONTAM86 and CONTAM87 developed by Dr. James Axley.

PB92-116805 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Gas and Particulate Science Div. New Way to Mount Particulate Material for Laser Microprobe Mass Analysis. Final rept.

R. A. Fletcher. 1989, 4p Pub. in Analytical Chemistry 61, n8 p**9**14-917 198**9**.

Keywords: \*Particulates, \*Carbon, \*Sample preparation, Quartz, Fibers, Aerosols, Air pollution, Mass spectroscopy, Reprints, Laser microprobe.

A new particle mounting sample preparation technique for the Laser Microprobe Mass Analyzer is presented. The substrate is high purity quartz fiber material conventionally used to collect airborne particulate matter. Advantages to using quartz fiber are low contamination, ease of sample preparation, and low background due to the transparency and high melting point of the

100.912

PB92-126630

(Order as PB92-126614, PC A06/MF A02) National Inst. of Standards and Technology, Gaithersbura, MD.

Accurate and Precise Coulometric Determination of Sulfur Dioxide in Compressed Gas Mixtures.

G. D. Mitchell, and A. A. Bell. 1991, 6p Included in Jnl. of Research of the National Institute of Standards and Technology, v96 n5 p541-546 Sep/Oct

Keywords: \*Voltametry, \*Air pollution detection, \*Chemical analysis, \*Sulfur dioxide, Acid rain, Gas cylinders, Compressed air, Binary mixtures, Performance evaluation, Standards, Electrochemistry, Comparison, Concentration(Composition), \*Standard reference materials.

Sulfur dioxide (SO2) in the atmosphere is a common pollutant and is a major contributor to the formation of acid rain. Accurate and precise determinations of SO2 in the atmosphere are essential to determine the magnitude of the problem. Reference gas mixtures such as NIST SRMs are an important part of the measurement procedure. Coulometry has been established as an important and reliable method for the determination of acidic compounds. The analytical method and simple apparatus described here are applied to the precise and accurate determination of sulfur dioxide in nitrogen, specifically in compressed gas cylinders at nominal concentrations of 50 and 100 micromol/mol (ppm). The method is constant current coulometry where the magnitude of the current is set by the balance between the electrochemical generation of OH(-), the flow of SO2, and the chemical reaction of the solution. The method is direct, rapid, and can be refined further to provide analysis at the nanomol/mol level.

100,913

PB92-126648

(Order as PB92-126614, PC A06/MF A02) National Inst. of Standards and Technology, Gaithersburg, MD.

Development of a Coulometric Method for Assessing the Concentration of Ambient Levels of CO2/ Air in Compressed Gas Mixtures.

G. D. Mitchell, and A. A. Bell. 1991, 4p Included in Jnl, of Research of the National Institute of Standards and Technology, v96 n5 p547-550 Sep/Oct

Keywords: \*Air pollution detection, \*Chemical analysis, \*Carbon dioxide, \*Voltametry, \*Voltametry, Concentration(Composition), Greenhouse effect, Comparison, Standards, Performance evaluation, Nondispersive infrared spectroscopy, Experimental design, Binary mixtures, Compressed air, Gas cylinders, \*Standard reference materials.

The understanding of global 'greenhouse' issues as they relate to CO2 in the atmosphere is a current environmental concern. At the National Institute of Standards and Technology there is a continuous search for methods of analysis that yield results that are traceable to fundamental quantities. The coulometric method presented here is a reliable method for the direct analysis of CO2/air cylinder gas mixtures. It is based on Faraday's laws of electrolysis and therefore no external standardization is required. A series of CO2/air cylinder gas mixtures ranging in concentration from 300 to 375 micromol/mol (ppm) were analyzed and the results compared to those results obtained by non-dispersive infrared (NDIR) analysis with traceability to gravimetric standards. The coulometric method is rapid, sensitive, precise, and with the proper experimental controls, will yield accurate results.

## **Environmental Health & Safety**

#### **Environmental Health & Safety**

100,914

PC A07/MF A02 PB92-116359 National Inst. of Standards and Technology (MEL), Gaithersburg, MD.
Response of Personal Noise Dosimeters to Con-

tinuous and Impulse-Like Signals.

Trudus and Impulse-Like Signals.
Technical note (Final).
D. J. Evans, D. R. Flynn, V. Nedzelnitsky, and E. D.
Burnett. Jun 91, 148p NIST/TN-1286
Also available from Supt. of Docs. as SN003-003-03116-0. See also PB80-176084 and PB86-109139.
Sponsored by Occupational Safety and Health Administration, Washington, DC.

Keywords: \*Personnel dosimetry, \*Dosimeters, \*Noise meters, \*Occupational safety and health, Keywords: \*Sound level meters, Occupational exposure, Regulations, Law enforcement, Design criteria, Performance evaluation, Continuous noise, Pulses, Signal-to-noise ratio, Standards, Calibrating, Acoustic detection, Sound intensity.

A study of the capabilities of noise dosimeters to measure personal exposure to time-varying and impulse-like noises was carried out. Ten commercial noise dosimeters were obtained. A laboratory reference noise dosimeter was constructed to provide a demonstrably accurate basis with which to compare the commercial noise dosimeters. Each commercial dosimeter, when ordered from the manufacturer, was specified to have: (1) a threshold A-weighted sound level of 80 dB, (2) a criterion sound level of 90 dB, and (3) an exchange rate of 5 dB and/or 3 dB. The performance of the commercial dosimeters was compared with theory and with results obtained from the reference dosiméter. Except in a few isolated cases, the commercial dosimeters were in general agreement with the performance specification of the appropriate American National Standard and with OSHA regulations

Solid Wastes Pollution & Control

100.915

PC A09/MF A02 DE91018580 Institute of Paper Science and Technology, Atlanta, GA. Chemical Recovery Group.

Fundamental studies of black liquor combustion. Report No. 4, Phases, 2, 3, and 4: Final report, December 1987--December 1989.

D. T. Clay, S. J. Lien, T. M. Grace, C. A. Brown, and H. L. Empie. Mar 90, 190p DOE/CE/40637-T9 Contract AC02-63CE40637

Sponsored by Department of Energy, Washington, DC.

Keywords: \*Black Liquids, \*Paper Industry, Boilers, Cogeneration, Combustion Properties, Energy Conservation, Energy Recovery, Furnaces, Mathematical Models, Progress Report, Waste Product Utilization, EDB/320303, EDB/320304.

The fundamentals of black liquor combustion are being studied in a project being carried out for the US Department of Energy by the Institute of Paper Science & Technology (IPST, formerly the Institute of Paper Chemistry) and the National Institute of Science & Technology (NIST, formerly the National Bureau of Standards). The project was divided into four phases. This report covers the completion of Phase 1 (in-flight processes), the results of all of the work on Phase 2 (char bed processes), Phase 3 (fume processes), and Phase 4 (furnace simulation). 41 refs., 62 figs., 30 tabs.

100,916

PB91-147264 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Chemical Thermodynamics Div.

NBS Research Program in Municipal Solid Waste Combustion.

Final rept. 1 Oct 85-30 Jun 86.

E. S. Domalski. 1986, 28p Sponsored by Department of Energy, Washington, DC. Biofuels and Municipal Waste Technology Div.

Pub. in Proceedings of Biofuels and Municipal Waste Technology Division Management Review Meeting, Washington, DC., July 29-30, 1986, 28p.

projects, Free radicals, Calorimeters, Reaction kinetics, Thermodynamics, Solid waste disposal.

Research activities conducted at NBS for DOE are summarized, covering the period 1 October 1985 to 30 June 1986. Major accomplishments consist of: (1) reporting of research results (8 publications), (2) describing modifications to the calorimeter's combustor, (3) studying reaction kinetics using H atoms and OH radicals as reactants, and (4) conducting combustion measurement which more closely simulate field conditions of real-world incinerators.

100,917

PB91-174631 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Chemical Thermodynamics Div.

Monitoring the Fate of Chlorine from MSW Sampling through Combustion. Final rept.

E. S. Domalski, K. L. Churney, A. E. Ledford, S. S. Bruce, T. J. Buckley, R. M. Parris, and S. N. Chesler. 1986, 14p

Pub. in Proceedings of Municipal Solid Waste as a Utility Fuel, Madison, WI., November 20-22, 1985, p16-1-16-14 1986.

\*Chlorine, \*Solid wastes, \*Municipal Keywords: wastes, Chemical analysis, Combustion, Field tests, Monitoring, Reprints, Baltimore County(Maryland), Brooklyn(New York).

The total chlorine and water soluble chlorine contents of the components of municipal solid waste (MSW) have been determined from sampling studies carried out at two sites, Baltimore County, MD, and Brooklyn, NY, for a five-day period. The total chlorine contents of the MSW samples from Baltimore County, MD, and Brooklyn, NY, are 0.45 and 0.89 mass %, respectively.

Keywords: \*Solid wastes, \*Combustion, \*Research

Replicate Measurements in the Interpretation of Environmental Monitoring.

Final rept.

W. S. Liggett. 1990, 7p Pub. in Environmental Monitoring, Restoration, and Assessment (What Have We Learned), p249-255

Keywords: \*Environmental monitoring, \*Replicating, Measurement, Errors, Probability density functions, Estimating, Analysis of variance, Sampling, Reprints.

In simultaneous monitoring at several sites, replicate samples and measurements, when chosen properly, provide a useful and unambiguous basis for data inter-pretation. Simultaneous monitoring permits calculation of indices of environmental change that are not influenced by weather changes. When the small changes measured by such an index are of interest, comparison of the index with the sampling and measurement error is appropriate. This comparison is made possible by the replicates. The familiar two-way table obtained by sampling a set of locations at several times is also considered. The indices considered are ones that perform well when large errors are more frequent than predicted by the normal distribution. Through the use of repli-cates, the variation in such indices caused by error alone can be assessed and thus environmental change is determined.

# INDUSTRIAL & MECHANICAL ENGINEERING

## Water Pollution & Control

100 918

Not available NTIS PB91-195040 National Inst. of Standards and Technology (IMSE), Gaithersburg, MD. Polymers Div. Simultaneous Butyltin Determinations in the Mi-

crolayer, Water Column and Sediment of a North-ern Chesapeake Bay Marina and Receiving System.

Final rept

C. L. Matthias, S. J. Bushong, L. W. Hall, J. M. Bellama, and F. E. Brinckman. 1988, 6p Pub. in Appl. Organomet. Chem. 2, n6 p547-552 1988.

Keywords: \*Chesapeake Bay, \*Water pollution, \*Metal alkyl compounds, Sediments, Estuaries, Marinas, Antifouling coatings, Toxic substances, Biodeterioration, Reprints, \*Tributyltins, Microlayers.

Butyltins were determined in the microlayer, water column and sediment of a northern Chesapeake Bay marina and its receiving system. Concentrations of the toxicant species tributyltin (TBT) ranged from 60 to 4130 ng/L in the microlayer, from 34 to 367 ng/L in the water column and from 0.05 to 1.4 microgram/g (dry weight) in sediment. TBT concentrations in all three environmental compartments were higher in the mari-nas than in the receiving system. Concentrations of TBT in the micro-layer and water column of the study area were potentially toxic to sensitive aquatic biota The microlayer appears to be depleted in dibutyltin relative to both water column and sediment, suggesting that the rate of stepwise dealkylation of dibutyltin is faster in the microlayer than in the other compartments studied.

## General

100,919

Not available NTIS PB91-189761 National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Statistical Engineering Div.

#### **Hydraulic & Pneumatic Equipment**

100,920

Not available NTIS PB91-134411 National Bureau of Standards (NEL), Gaithersburg,

MD. Chemical Process Metrology Div. Flowmeter Installation Effects: A New Approach to an Old but Prevalent Problem.

Final rept. G. E. Mattingly, and T. T. Yeh. 1986, 22p See also PB89-132856.

Pub. in Proceedings of International Conference on Flow Measurement in the Mid 80's, East Kilbride, Glasgow, June 9-12, 1986, p1-22.

Keywords: \*Pipe flow, \*Flow measurement, \*Flow visregulation, Flowmeters, Velocity measurement, Fluid flow, Turbulent flow, Pipes(Tubes), Reprints, Laser doppler velocimeters, Velocity distribution.

For a selected piping configuration, elbows-out-ofplane, preliminary results are presented for laser Doppler velocimetry (LDV) profiles taken in the down-stream piping near tis configuration. These results quantify pipeflow profiles for both time-averaged and turbulent-velocity components as well as swirl-angle and power-spectral density distributions. It is planned that these experiments will describe the pipeflows downstream of this configuration. These results are also intended to provide validation data for computer modelling studies of this flow. It is also planned that future phases of this research include pipeflows from other prevalently encountered piping configurations. Additionally, these phases can also focus on the benefit-cost aspects (capital and pressure loss) of flow-conditioning elements.

100,921

PB91-134445 Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Chemical Engineering Science Div. Effect of the Location of an In-Line Tube Bundle

111

on Orifice Flowmeter Performance. Final rept. S. E. McFaddin, C. F. Sindt, and J. A. Brennan.

1989, 6p Contract GRI-5081-353-0422

Sponsored by Gas Research Inst., Chicago, IL. Pub. in Flow Meas. Instrum. 1, p9-14 Oct 89.

## INDUSTRIAL & MECHANICAL ENGINEERING

## **Hydraulic & Pneumatic Equipment**

Keywords: \*Orifice meters, \*Flowmeters, \*Orifice flow, Finishes, Flow measurement, Fluid flow, Surface properties, Reprints, \*Rod bundles, Discharge coefficient.

The Gas Research Institute has sponsored many significant flow measurement studies at the National Institute of Standards and Technology. The main thrust of the 1988 research project was to determine the effect of the location of an in-line tube bundle flow conditioner on the orifice discharge coefficient. An in-line tube bundle was placed at four locations-7, 12, 17, and 27 pipe diameters upstream of the orifice plate in a 100mm (4 inch) orifice meter. The research has determined that if the in-line tube bundle is placed at 7 pipe diameters, the minimum distance specified in the flow measurement standards for a 0.75 beta ratio plate, as much as 1% error in the discharge coefficient occurs. At 17 pipe diameters, the discharge coefficients of all the beta ratios are statistically the same as would be determined in 'ideal' conditions. These new experimental data will help to improve the current flow measurement standards and suggest the direction of future research.

100.922 PB91-147108 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Center for Chemical Technology. Stabilization Techniques for Spinning Rotor Gage Residual Drag. Final rept.

S. H. Choi, S. Dittmann, and C. R. Tilford. 1990, 7p Sponsored by Department of Energy, Washington, DC.

Office of Fusion Energy.
Pub. in Jnl. of Vacuum Science and Technology A 8, n6 p4079-4085 Nov/Dec 90.

Keywords: \*Vacuum gages, Rotor dynamics, Stabilization, Measurement, Instability, Reprints, Residual drag.

The pressure-independent residual drag on a spinning ball requires an offset correction for the accurate use of a spinning rotor vacuum gage (SRG) at low pres-sures. Instabilities in the residual drag (RD) can cause significant errors in low-pressure SRG measurements. The instabilities usually occur as discontinuous shifts when a ball is levitated by the magnetic suspension, or as continuous changes as the ball slows down. The discontinuous shifts in residual drag have been found to be caused by changes in the orientation of the ball's magnetic moment, induced by the suspension field or the inductive drive circuit. Premagnetizing the ball in a strong field has stabilized the orientation of the magnetic moment and the RD value. The continuous changes are caused by competition between magnetic and inertial forces, which result in a frequency-dependent orientation of the rotational axis of the ball. Etching a spot on the ball alters its shape and defines an inertial axis. Magnetizing the ball in a preferred direction with respect to the axis minimizes both the residual drag and its frequency dependence.

100.923 PB91-147488 Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Chemical Engineering Science Div. SHOOT Flowmeter and Pressure Transducers. Final rept.

A. Kashani, R. A. Wilcox, A. L. Spivak, D. E. Daney, and C. E. Woodhouse. 1990, 6p Pub. in Cryogenics 30, p286-291 Mar 90.

\*Pressure transducers, \*Flowmeters, Keywords: Spaceborne experiments, Liquid helium, Superfluidity, Reprints, SHOOT experiment.

A venturi flowmeter has been designed and constructed for the Superfluid Helium On-Orbit Transfer (SHOOT) experiment. The calibration results obtained from the SHOOT venturi demonstrate the ability of the flowmeter to meet the requirements of the SHOOT experiment. Flow rates as low as 20 cu dm/h and as high as 800 cu dm/h have been measured with the flowmeter. The pressure drop in the flowmeter is measured by two Validyne differential pressure transducers. The ranges of the two transducers are 0.86 kPa (0.125 p.s.i.d.) and 8.62 kPa (1.25 p.s.i.d.). The low range transducer measures flow rates less than 200 cu dm/ h, whereas the high range transducer measures flow rates greater than 200 cu dm/h. The repeatability of the flowmeter at the nominal flow rate of 500 cu dm/h is within + or - 1% of the flow rate. Performances of the SHOOT differential and absolute pressure transducers, which have undergone calibration and vibration tests, are also included. Throughout the tests, the responses of the transducers remained linear and repeatable to within + or - 1% of the full scales of the transducers

#### Laboratory & Test Facility Design & Operation

100,924 N91-21361/1

(Order as N91-21331/4, PC A24/MF A03) National Inst. of Standards and Technology (NML), Gaithersburg, MD. Thermophysics Div. High-Speed Spatial (Linear) Scanning Pyrometer: A Tool for Diagnostics, Temperature Mapping, and

Property Determinations at High Temperatures. A. Cezairliyan, R. F. Chang, and G. M. Foley. 1 May

90, 5p In JPL, Proceedings of the First Workshop on Contain-in Microgravity p 352-356.

Keywords: High temperature environments, \*Pyrometers, Scanners, Temperature distribution, \*Temperature measurement, Linear arrays, Photodiodes, Radiance, Reduced gravity, Silicon, Spectra.

Development of a fast spatial scanning pyrometer for temperature measurements above 1500 K is described. The salient features of the pyrometer are: (1) it measures spectral radiance temperature (at 0.65 micron) at 1024 points along a straight line (25 mm long) on the target; (2) it has no moving parts and uses a self-scanning linear array of silicon photodiodes as the detector; (3) its output is recorded digitally every 1 microsec with a full-scale resolution of about 1 part in 4000, permitting performance of a complete cycle of measurements (1024 points) in about 1 ms. Operationall characteristics of the pyrometer are given. Examples of measurements of the temperature along rapidly heated (resistive self-heating) specimens (rod, tube, strip) are presented. Potential use of the pyrometer in the experiments, both ground-based and in microgravity, requiring temperature mapping and property distribution of the specimen at high temperatures is discussed.

PC A04/MF A01 PB91-132282 National Inst. of Standards and Technology (MSEL), Boulder, CO. Materials Reliability Div. Data-Reduction and Analysis Procedures Used in NIST's Thermomechanical Processing Research. Y. W. Cheng, and C. L. Sargent. Aug 90, 68p NISTIR-3950

Keywords: \*Computer systems programs, \*Data processing, Data reduction, Phase transformations, Test equipment, Deformation, Strain rate, Loads(Forces), Cooling rate, Time dependence, \*Thermomechanical treatments, Temperature dependence.

The report described the data-reduction procedures and computer programs used to reduce and analyze the data obtained with a hot-deformation apparatus. The measured raw data with the apparatus include temperature vs. time, specimen's relative length (dilation) vs. time, actuator movement (stroke) vs. time, and load vs. time. Four computer programs were writ-ten for data reduction and analysis to determine the cooling rates, the true stress-true strain curves, the true strain rates, and the phase-transformation temperatures. Local averaging techniques were used to smooth the data of temperature, dilation, stroke, and load. Source codes for the computer programs are included. Example results of the analyses are presented and an example of the program execution is given.

PB91-147272 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Thermophysics Div.
Study of the Linearity of Transfer Leaks and a Helium Leak Detector. Final rept.

C. D. Ehrlich, S. A. Tison, H. Y. Hsiao, and D. B. Ward. 1990, 6p Pub. in Jnl. of Vacuum Science and Technology A 8, n6 p4086-4091 Nov/Dec 90.

Keywords: \*Leak detectors, \*Linearity, Helium, Leakage, Gas detectors, Flow measurement, Accuracy, Errors, Drift(Instrumentation), Mass spectrometers, Random variables, Reprints.

A study has been performed of the linearity of two types of variable-reservoir-pressure leaks and a commercial tuned magnetic sector mass-spectrometer helium leak detector. While the leaks exhibit predict-able (but not always linear) behavior over a broad range, the linearity of the leak detector depends strongly on properly correcting for observed drift and random fluctuations in the measured leak rate.

100.927

PB91-158519 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Inorganic Materials Div. Levitation Calorimetry

Final rept.

D. W. Bonnell, R. L. Montgomery, B. Stephenson, P. C. Sundareswaran, and J. L. Margrave. 1988, 34p Sponsored by Rice Univ., Houston, TX. Dept. of Chem-Pub. in Specific Heat of Solids, p265-298 1988

Keywords: \*Calorimetry, \*Leviation melting, \*Liquid metals, Specific heat, Thermodynamic properties, High temperature tests, Heat measurement, Reviews,

The determination of high temperature thermodynamic properties is of fundamental importance in chemistry, physics, and engineering. The temperature region above 2000 K has been generally inaccessable to direct measurement, with basic properties even of elements often being obtained by extrapolation. The development of levitation calorimetry has provided the technique for precision measurements of conducting technique for precision measurements of conducting materials in the previously difficult to study regime. The chapter presents a review of the development of the field, from the first successful calorimeter system in the late 1960's, to the reviewed, and the various considerations in coil development are discussed. Actual calorimeter systems are discussed, with a detailed development of the data analysis being presented. A comprehensive review of the literature is presented, with examples of results obtained and comparisons of the current state of liquid properties.

100 928

PB91-159004 Not available NTIS National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Metallurgy Div. Mechanical Testing Revitalized. Final rept.

L. Mordfin. 1990, 1p

Pub. in Experimental Techniques 14, n5 p20 Sep/Oct

Keywords: \*Mechanical tests, \*Strain gages, Test fa-cilities, Stress analysis, Strain measurement, Mechani-cal properties, Nondestructive tests, Experimentation, Materials testing, Reprints.

The fiftieth anniversary of the invention of the bonded The fiftieth anniversary of the invention of the bonded resistance strain gage was celebrated last year. Over a period of about twenty years, which encompassed World War II and the postwar years, this device completely revolutionized the field of experimental stress analysis. Today, this field is considered relatively mature; although strain gages continue to be used in ever-increasing quantities, significant new advantage and the way they are used have become rare. ments in the way they are used have become rare. The field of mechanical testing, which is closely intertwined with that of experimental stress analysis, grew in much the same way. . . until the 1980s. The last ten years have witnessed a revival of interest in mechanical testing, with major efforts devoted to the development of new mechanical test methods and techniques to satisfy needs for new kinds of measurements on new kinds of materials. A new group on Mechanical Properties and Performance was established at NIST to address these needs. It is suggested that the Society for Experimental Mechanics could fulfill an important role as a central forum for the revitalized field of mechanical testing.

100.929

PB91-175067 Not available NTIS PB91-17506/
National Inst. of Standards and Technology (IMSE),
Gaithersburg, MD. Ceramics Div.
High-Resolution Small-Angle X-ray Scattering
Camera for Anomalous Scattering.

Final rept. G. G. Long, P. R. Jemian, J. R. Weertman, D. R. Black, H. E. Burdette, and R. Spal. 1991, 8p Sponsored by Department of Energy, Washington, DC.

# **INDUSTRIAL & MECHANICAL ENGINEERING** Laboratory & Test Facility Design & Operation

Pub. in Jnl. of Applied Crystallography 24, p30-37

Keywords: \*Small angle scattering, \*Cameras, \*X-ray analysis, \*Photodetectors, Test equipment, Measuring instruments, Steels, Microstructure, Temperature de-pendence, Photodiodes, Precipitates, Calibrating, AC generators, Correlators, Reprints.

The design and operation of a new small-angle X-ray scattering instrument, optimized for high throughput at a synchrotron source, high angular and wave-length resolution, large sample cross-sectional area, accurate energy tuning, excellent signal-to-noise ratio and rate energy tuning, excellent signal-to-noise ratio and harmonic rejection are presented. The principles of design and implementation are given, as are the details of primary calibration of absolute intensity and experimental desmearing. The instrument has been tested for application to anomalous-scattering measurements near the chromium K edge. Preliminary results on samples of a heat-treated steel are presented as a demonstration of the capability of this experiment to separate the microstructure evolution as a function of temperature of a chromium-rich precipitate from the thermal behavior of other precipitates in the steel.

PB91-175216 Not available NTIS National Inst. of Standards and Technology (MSEL), Boulder, CO. Fracture and Deformation Div.

Jlc Data Analysis with a 'Negative Crack Growth' Correction Procedure.

Final rept.

Y. A. Rosenthal, R. L. Tobler, and P. T. Purtscher. 1990, 4p

Pub. in Jnl. of Testing and Evaluation 18, n4 p301-304 Jul 90.

Keywords: \*Crack propagation, \*J integral, \*Mechanical tests, Crack initiation, Fracture mechanics, Austenitic steels, Measurement, Standards, Fracturing, Fracture properties, Toughness, Reprints.

It often occurs in J-R testing that some of the initial crack extension data points have anomalous negative values. ASTM Methods 813-87 and 813-81, however, do not specify any procedures for treating such data. The authors propose a procedure for data analysis which utilizes the negative data point values and is consistent with ASIM E 813-87. The proposed correction procedure is illustrated using a data set for austen-itic steel; also, J values obtained using ASIM E 813-87 are compared to those obtained from its predecessor E 813-81.

100,931 PB91-175406 Not available NTIS Mational Bureau of Standards (NEL), Gaithersburg, MD. Mechanical Production Metrology Div. Eccentric Load Sensitivity of Force Sensors. Final rept.

R. A. Mitchell, R. L. Seifarth, and C. P. Reeve. 1986,

Pub. in Mechanical Problems in Measuring Force and Mass, p275-281 1986.

Keywords: \*Force, \*Sensors, \*Eccentricity, Loads(Forces), Measurement, Statistical analysis, Mathematical models, Tension, Compressive proper-ties, Bending moments, Sensitivity, Reprints.

A test has been developed to measure the eccentric load sensitivity of universal (tension and compression) force sensors. The test can also be used to calibrate the transverse bending moment measuring bridges of multi-axis force-moment sensors. Results of tests of five sensors are given. The results are analyzed in terms of a sinusoidal statistical model.

100,932 PB91-187633

(Order as PB91-187617, PC A06/MF A01) National Inst. of Standards and Technology, Gaithers-

burg, MD.
Use of the Electrostatic Classification Method to Size 0.1 micrometer SRM Particles: A Feasibility

Study.
P. D. Kinney, D. Y. H. Pui, G. W. Mulholland, and N. P. Bryner. 1991, 30p

Sponsored by Minnesota Univ., Minneapolis. Included in Jnl. of Research of the National Institute of Standards and Technology, v96 n2 p147-176 Mar/Apr

Keywords: \*Dimensional measurement, \*Particle size, \*Microspheres, Aerosol generators, Atomizers, Con-

densation nuclei, Polystyrene, Electrostatics, Mobility, Feasibility, \*Standard reference materials.

The use of the electrostatic classification method for sizing monodisperse 0.1 micrometer polystyrene latex (PSL) spheres has been investigated experimentally. The objective was to determine the feasibility of using electrostatic classification as a standard method of particle sizing in the development of a 0.1 micrometer particle diameter Standard Reference Material (SRM). The mean particle diameter was calculated from a measurement of the mean electrical mobility of the PSL spheres as an aerosol using an electrostatic classifier. The performance of the classifier was investigated by measuring its transfer function, conducting a sensitivity analysis to verify the governing theoretical relationships, measuring the repeatability of particle sizing, and sizing NIST SRM 1691, 0.269 micrometer and NIST SRM 1690, 0.895 micrometer particles.

100,933 PB91-206730 PC A03/MF A01 National Inst. of Standards and Technology (BFRL), Gaithersburg, MD.

Calibration at 24C of a Heat-Flow-Meter Apparatus Having 610 mm Square Plates. R. R. Zarr, and B. A. Licitra. May 91, 36p NISTIR-

4539

Sponsored by Department of Energy, Washington, DC. Office of Buildings Energy R and D.

Keywords: \*Heat flow meters, \*Calibration, Heat measurement, Heat flux, Heat transmission, Test facili-ties, Plates, Data acquisition, Thermal insulation, Ther-mal measurements, Thermal conductivity.

Results are summarized for 38 individual calibration measurements conducted at 24 C and atmospheric conditions for a heat-flow-meter apparatus having 610 mm square plates. The apparatus was calibrated using a 26.2-mm-thick specimen of fibrous-glass board having a density of 139 kg/cu m. The specimen was selected from an internal lot (Lot 1970) of Standard Reference Material (SRM) similar to SRMs 1450, 1450a, and 1450b. Values of apparent thermal conductivity was excellent of the standard services a segregation of the standard services are services. ductivity were predicted using a regression equation developed for the lot of fibrous-glass insulation. Calibration measurements varied + or - 0.4% with small drift of 0.4% over 250 days. The apparent thermal conductivity of the calibration specimen was also measured using the National Institute of Standards and Technology's one-meter Line-Heat-Source Guarded Hot Plate. Agreement between measurements of thermal conductivity of the guarded hot plate and predicted values were within +0.2 to -0.3% at 24 C. The report describes the heat-flow-meter apparatus and the computer data-acquisition-system used to collect data from the apparatus.

100,934

PB91-222646 PC A08/MF A02 National Inst. of Standards and Technology (TS), Gaithersburg, MD.

Directory of Accredited Laboratories, 1991. Nabirectory of Accredited Laboratories, 1991. National Voluntary Laboratory Accreditation Program (NVLAP). Final rept. N. M. Trahey, V. R. White, and J. Horlick. Apr 91, 1709 NIST/SP-810

Also available from Supt. of Docs. as SN003-003-03082-1. See also PB90-198920.

Keywords: \*Laboratories, \*Directories, Acoustics, Asbestos, Carpets, Computer applications, Construction materials, Dosimetry, Electromagnetic compatibility, Paints, Papers, Plastics, Sealers, Seals(Stoppers), Stoves, Telecommunication, Thermal insulation, \*National Voluntary Laboratory Accreditation program, NVLAP program.

The annual Directory provides a listing of laboratories accredited as of March 1, 1991, by the National Institute of Standards and Technology, National Voluntary Laboratory Accreditation Program (NVLAP). The names of approximately 900 laboratories in 15 fields of testing are included. A brief description of the NVLAP program is given, and a summary of laboratory participation is provided. To aid the user indexes core references. pation is provided. To aid the user, indexes cross reference the laboratories by company name, NVLAP Lab Code Number, field of testing, and geographic location (state or country). A listing of the test methods (scope of accreditation) is provided for each laboratory.

100,935 PB92-109024

PC A03/MF A01

National Inst. of Standards and Technology (CSTL), Gaithersburg, MD. Process Measurements Div.

Procedure for the Effective Recalibration of Liquid-in-Glass Thermometers.

Special pub. (Final). J. A. Wise. Aug 91, 19p NIST/SP-819 Also available from Supt. of Docs. as SN003-003-

Keywords: \*Temperature measuring instruments, \*Thermometers, \*Calibration, Volume, Liquid in glass thermometers, Ice baths, ITS-90.

High quality liquid-in-glass thermometers require only one complete calibration in their lifetime and it is possible to avoid the usual requirement for complete recalibration of the instrument by the recalibration of a single previously calibrated temperature. The need for recalibration of properly manufactured liquid-in-glass thermometers is due to the gradual relaxation of residual mechanical strains in the glass that have a significant effect on the volume of the bulb. The recalibration of a single point provides a reliable indication of the effect of this change in volume and provides a means for the accurate adjustment of the remainder of the scale. The paper describes a procedure for the single temperature recalibration of liquid-in-glass thermom-eters that can be performed in the user's laboratory and the subsequent adjustment of the entire scale. The adjustment of the scale that is required by the recent introduction of the new International Temperature Scale (ITS-90) is also described.

100.936

03102-0

PB92-126416 PC A10/MF A03 National Inst. of Standards and Technology (TS), Gaithersburg, MD. Physical Measurement Services

Program.

NIST Calibration Services Users Guide, 1991.

J. D. Simmons. Oct 91, 221p NIST/SP-250 91ED Also available from Supt. of Docs. as SN003-003-03115-2. Supersedes PB89-200216. See also PB90-127820.

Keywords: \*Fees, \*Metrology, Manual, Measuring instruments, Test facilities, Standards, Dimensions, Mechanical tests, Acoustics, Ultrasonics, Microwaves, Thermodynamics, Ionizing radiation, Electromagnetic properties, Prices, \*National Institute of Standards and Technology, \*Calibration.

The National Institute of Standards and Technology (NIST) Calibration Services Users Guide provides de tailed descriptions of currently available NIST calibration services, measurement assurance programs, and special test services. The following measurement areas are covered: (1) dimensional; (2) mechanical, including the programs of the control o cluding flow, acoustic, and ultrasonic; (3) thermodynamic; (4) optical radiation; (5) ionizing radiation; and (6) electromagnetic, including dc, ac, rf, and microwave. A separate Fee Schedule is issued annually, providing current prices for the services offered, updates on points of contact, and information on measurement seminars.

100,937

PB92-126655

(Order as PB92-126614, PC A06/MF A02) National Inst. of Standards and Technology, Gaithers-

burg, MD. Certification of NIST SRM 1961: 30 micrometers Di-

ameter Polystyrene Spheres.
A. W. Hartman, T. D. Doiron, and G. G. Hembree.
1991, 13p
Included in Jnl. of Research of the National Institute of

Standards and Technology, v96 n5 p551-563 Sep/Oct

Keywords: \*Dimensional measurement, \*Particle size, \*Microspheres, Electron microscopy, Optical microscopy, Polystyrene, \*Standard reference materials.

The report describes the certification of SRM 1961, an NIST Standard Reference Material for particle diameter. It consists of an aqueous suspension of monosize 30 micrometers diameter polystyrene spheres. The primary technique used optical microscopy; it gave a mean diameter value D(bar) = 29.62 + or - 0.04 micrometer and a standard deviation of the size distribution of 0.21 micrometer. Over 2000 spheres were measured. The supporting technique used electron microscopy, which yielded D(bas) = 29.68 + or - 0.11 micrometer. Ninety spheres were measured.

100,937

## **INDUSTRIAL & MECHANICAL ENGINEERING**

## Laboratory & Test Facility Design & Operation

100,938 PB92-126721

(Order as PB92-126614, PC A06/MF A02) Slovak Metrological Society, Bratislava (Czechoslovakia).

Slovak Metrologicai Society.

J. Mandak. 1991, 2p Included in Jnl. of Research of the National Institute of Standards and Technology, v96 n5 p621-622 Sep/Oct

Keywords: \*Metrology, Czechoslovak organizations, Historical aspects, Meetings, \*Slovak Metrological Society.

The brief communication describes the establishment of the Slovak Metrological Society (SMS). SMS came into being on October 16, 1990, as the result of a special founding Congress held in DT Zilina with 137 delegates from the whole of Slovakia in attendance. It brings together individuals involved in both the technical and legal aspects of metrology and its aim is to help in developing metrology and measurement in Slovakia. SMS functions under the direction of the Czechoslovak Metrological Institute (CSMU), the center of Czechoslovak metrology. Together with the Federal Weights and Measures Office (FUNM), state metrological centers, centers of the calibration service, and production plant metrological centers, it establishes the principal tasks of present-day metrology in the Czechoslovak Federal Republic (CSFR).

100,939 PB92-163864 Not available NTIS National Inst. of Standards and Technology (TS), Gaithersburg, MD. Physical Measurement Services Program.
Modernized Metric System (Chart).

Aug 91, 1p NIST/SP-304-91-ED

Keywords: \*Metric system, Units of measurement, Training aids, Metric system, SI, Units of measurement.

The chart presents a popularized yet technically accurate guide to SI base units, supplementary units, multiples and prefixes, and common conversions. The intended audience is (mainly) school children and the general public.

PB92-163872 Not available NTIS National Inst. of Standards and Technology (TS), Gaithersburg, MD. Physical Measurement Services

Brief History of Measurement Systems with a Chart of the Modernized Metric System. Aug 91, 1p NIST/SP-304A-91-ED

Keywords: \*Metric system, International system of units, Measurement, History.

The Modernized Metric System (also called the International System of Units) is made up of seven base units, two supplementary units, and many derived units. The chart describes this entire system, including details about the standards for each base unit and information on how the system is used. The reverse side of the chart contains a brief history of measurement systems. The need for measurement began with primative man, who used parts of his body and his natural surroundings for measurement standards and measuring instruments. As societies evolved, weights and measures became more complex. Two systems became predominant: the English system, rooted in the history and tradition of England; and the metric system, a scientifically based system using decimal notation. The metric system, with its inherent decimal advantages, gained widespread acceptance and is now the official measurement system in nearly all countries of the world.

100,941 PB92-163880 PB92-163880 Not available NTIS National Inst. of Standards and Technology (TS), Gaithersburg, MD. Physical Measurement Services Program

Metric Conversion Card. Final rept.

J. D. Simmons. Aug 91, 1p NIST/SP-365-91-ED

Keywords: Metric system, \*Metrication, Units of measurement.

NIST SP365 is a pocket size plastic Metric Conversion Card with approximate conversions to and from metric

for the most commonly used units of measurement on the opposite sides of the card.

100 942

PB92-163898 Not available NTIS National Inst. of Standards and Technology (TS), Gaithersburg, MD. Physical Measurement Services Program.

Metric Measures Up (Ruler). Final rept.

Aug 91, 1p NIST/SP-376-91-ED

Keywords: \*Units of measurement, Metric system.

This ruler provides metric linear measure (17.75) and customary-unit linear equivalents (approximately 7

#### **Manufacturing Processes & Materials** Handling

1*00,943* **PB92-126457** PC A05/MF A01 National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Polymers Div. Development of Test Methods to Determine the

Compatibility of Liquid Hazardous Materials with Polyethylene Packagings. Final rept. 11 Jun 90-31 Dec 91. J. M. Crissman, and M. A. Schen. Dec 91, 77p NISTIR-4729

Contract DTRS-56-90-X-70006

See also PB-280 215 and PB90-235417. Sponsored by Department of Transportation, Washington, DC. Office of Hazardous Materials Regulations

Keywords: \*Hazardous materials, \*Polyethelene,
Compatibility, Test methods, \*Shipping containers, Compatibility, Test methods, Packaging, Oxidation, Permeability, Cracks, Degradation, Peroxides, Transportation safety, Regulations, Hazardous materials transportation, Organic peroxides, Hazardous liquids.

The report describes work done for the Department of Transportation, Office of Hazardous Materials Transportation, to develop test methods which can be used to determine whether a liquid hazardous material may be shipped in a specific type of polyethylene container. Current federal regulations require that each prospective lading be tested individually in proposed polyethylene packagings. The central task of the project is to determine the feasibility of substituting a set of standard liquids for the purpose of compatibility testing with polyethylene. In determining the compatibility of haz-ardous liquids with polyethylene there are three major areas of concern, permeation and/or swelling, environmental stress cracking, and oxidative degradation. Specific recommendations are made for a set of standard liquids which address all three aspects of compatibility. Special attention is given the class of or-ganic peroxides which may be unstable at the test temperatures currently in use. In the area of permeation, an empirical method known as the 'Permachor' scheme is proposed as a means of estimating the permeability of many liquid hazardous materials, and for ranking individual members within a given class of liq-

## **Nondestructive Testing**

Not available NTIS PB91-187120 National Inst. of Standards and Technology (IMSE), Boulder, CO. Fracture and Deformation Div. Eddy Current Reflection Probe: Theory and Exper-Iment.

Final rept.

B. A. Auld, J. C. Moulder, S. Jefferies, P. J. Shull, and S. Ayter. 1989, 11p Pub. in Research in Nondestructive Evaluation 1, n1 p1-11 1989.

Keywords: \*Eddy currents, \*Nondestructive tests, Signal processing, Measuring instruments, Electric coils, Defects, Probes, Finite difference method, Reflection, Experimental data, Aluminum, Reprints.

Eddy current reflection probes are two-port devices consisting of a drive coil encircling a differential pair of

pickup coils. In operation, the drive coil is excited with an alternating current and the signal detected is the emf induced in the pickup coils. When no flaw is present there is no output signal, but when a flaw is present, the perturbed field from the drive coil induces a signal in the pickup coils. In this respect, reflection probes are fundamentally different from absolute eddy current probes, which are generally operated as pas-sive elements in a bridge circuit. With an absolute probe, the impedance of the probe is monitored and a flaw is detected by the change in probe impedance it causes. A general delta Z theory of eddy current reflection probes was previously developed for application to new types of robotic sensors. In the paper the theory is applied to the characterization of surfaceconnected flaws. Flaw signals were calculated using a finite-difference implementation of the delta Z theory developed at Stanford University. A special air-core eddy-current reflection probe was fabricated at NBS and used to obtain flaw signals for a number of rectangular-shaped slots in aluminum. An automatic impedance analyzer was used to measure flaw signals as the probe was scanned down the length of a flaw. The paper compares the experimental results with predictions of the theory.

100,945 PB91-236562 Not available NTIS National Inst. of Standards and Technology (EEEL), Boulder, CO. Electromagnetic Technology Div. Eddy Current Probe Sensitivity as a Function of Coil Construction Parameters. Final rept.

T. E. Capobianco, J. Splett, and H. Iyer. 1990, 18p Pub. in Res. Nondestr. Eval. 2, p169-186 1990.

Keywords: \*Nondestructive tests, \*Eddy current tests, \*Electric coils, Notch tests, Eddy currents, Defects, Permeability, Measuring instruments, Wire, Sensitivity, Inspection, Reprints.

The authors report the results of the first phase of a study designed to quantify the relationship between eddy current coil construction and the performance of these coils used in nondestructive evaluation (NDE) inspections. The ferrite core coils wound for the study are small but typical of the sizes commonly used in commercially manufactured eddy current probes. The data reported here were produced from a set of 27 probes scanned over a single defect. The defect was an electrical-discharge-machined (EDM) notch in a 19 mm thick 7075-T6 aluminum alloy specimen. The partcircular EDM notch was 9 mm long and 3 mm deep and 0.1 mm wide. Analysis of the data shows that the number of turns, the winding distance, the coil aspect ratio, and the backside ferrite length all affect the coil sensitivity. Winding inhomogeneity is significant for coils having many winding layers and can be considerably larger than the contribution made by variations in some of the construction factors. Wire gauge, ferrite diameter, and permeability showed no significant effects on their measure of sensitivity in the study.

PB91-237305 Not available NTIS National Inst. of Standards and Technology (IMSE), Boulder, CO. Fracture and Deformation Div. Characterization of Capacitive Array for NDE Applications. Final rept.

P. J. Shull, A. V. Clark, P. R. Heyliger, J. C. Moulder, and B. A. Auld. 1990, 17p Pub. in Research in Nondestructive Evaluation 2, p11-27 1990.

Keywords: \*Nondestructive tests, \*Capacitance, \*Dielectrics, \*Arrays, Detectors, Ferroelectric materials, Capacitors, Measuring instruments, Dielectric proper-

The authors have developed a capacitive array sensor which responds to the complex dielectric constant of an interrogated material. The sensor requires only single-sided access and operates in a differential mode for detection of discontinuities in the relative dielectric constant, or in the absolute mode where the interest is in absolute quantities. The device in general is noncontacting but can be fabricated as an embed-ded sensor. Various proof-of-concept studies have been performed to explore possible applications of the device. In the differential mode, small surface features (notches) were detected in a conductor, in dielectrics, both surface and subsurface features were detected. The probe was sensitive to change in impedance caused by a curing epoxy, viewed through a graphite-

# **INDUSTRIAL & MECHANICAL ENGINEERING**

## **Nondestructive Testing**

epoxy composite panel. A study was performed to assess the use of the probe for noncontact characterization of sintering of ceramics. In this (absolute) mode, the effects of liftoff and dielectric constant must be separated. They propose a scheme based on the ability to multiplex the capacitive array probe to accomplish this. Preliminary investigation shows that the effect of parasitic capacitance between the probe and ground points in the environment must be suppressed.

100,947 PB91-237313 Not available NTIS National Bureau of Standards (IMSE), Boulder, CO. Fracture and Deformation Div.

Capacitive Array Sensors for Nondestructive Evaluation.

Final rept. P. J. Shull, P. Heyliger, B. A. Auld, and A. V. Clark. 1988, 1p

Pub. in Jnl. of Metals 40, n11 p112 1988.

Keywords: \*Capacitance, \*Detectors, \*Nondestructive tests, \*Arrays, \*Ceramics, Dielectric materials, Sintering, Surface properties, Epoxy resins, Coatings(Materials), Defects, Insulators, Electric conductors, Reprints.

Capacitive array sensors can be used to characterize; (1) surface features on conductors; (2) surface and subsurface features on dielectrics. The versatility is a decided advantage over inductive probes. The study characterized the sensor on both conductors and dielectrics for a variety of both real and simulated surface and subsurface (dielectrics only) flaws. This was done with the probe elements configured for both absolute and differential modes. In the absolute mode there are two electrodes - a source and a receiver. A voltage is impressed across these elements. In the differential mode there are three electrodes: one source and two receiver electrodes. These receiver electrodes are then connected to a differential amplifier. The probe's potential was examined for the following applications: monitoring of the cure of epoxy resins, thickness and porosity of thermal barrier coatings, flaws in ceramics and subsurface flaws in insulators.

100,948 PB91-237610 Not available NTIS National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Materials Reliability Div.
Theory of Capacitive Probe Method for Noncon-

tact Characterization of Dielectric Properties of Materials.

V. K. Tewary, P. R. Heyliger, and A. V. Clark. 1991,

10p

Pub. in Jnl. of Materials Research 6, n3 p629-638 Mar

Keywords: \*Dielectric materials, \*Capacitance, Finite element analysis, Hilbert transformation, Reliability, Characterization, Nondestructive tests, Capacitance, Measurement, Monitors, Theories, Surface energy, Reprints, Capacitive probe.

The capacitive probe method for noncontact characterization and monitoring of dielectric materials is analyzed theoretically. An analytical method based upon the Hilbert transform technique and a numerical method using the finite element technique for calculating the potential distribution and change in admittance of the probe caused by presence of the dielectric ma-terial as a function of liftoff (distance between the probe plane and the surface of the dielectric material) are described. The two methods are compared with each other and their relative advantages discussed. The possibility of extracting useful information about the dielectric constant of the material from experimental data is also discussed in the light of the proposed theory.

100,949 PB92-117423 Not available NTIS National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Metallurgy Div.

Advanced Sensing of Materials Processing.

H. N. G. Wadley, A. H. Kahn, and W. L. Johnson.

1988, 10p

Pub. in Materials Research Society Symposium Proceedings, v117 p109-118 1988.

Keywords: \*Nondestructive tests, \*Process control, \*Metals, \*Detectors, Artificial intelligence, Reviews, Microstructure, Measurement, Ultrasonic tests, Acoustic emission, Eddy currents, Reprints.

To implement new process control strategies including Intelligent Processing of Materials, advanced sensors are required to nonintrusively evaluate process and mi-crostructure variables. Researchers increasingly are looking to innovative extensions of traditional nondestructive evaluation technologies, such as ultrasonics, acoustic emission, and eddy current methodologies for this. Here, the nature and characteristics of emerging sensors based upon these new measurement methods are described and examples of their application discussed.

# LIBRARY & INFORMATION **SCIENCES**

## **Information Systems**

100.950 PB91-157123 PC A03/MF A01 National Inst. of Standards and Technology, Gaithersburg, MD.
STEP On-Line Information Service User's Guide. National PDES Testbed Report Series. S. Katz. 2 Jan 91, 25p NISTIR-4491 Supersedes PB91-143354.

Keywords: \*Information services, \*On line systems, Information systems, Access methods, User manuals, Documents, Computer software, Computer networks, STEP(Standard for the Exchange of Product Model Data), PDES(Product Data Exchange using STEP), National Institute of Standards and Technology.

The document describes how to access the on-line STEP (Standard for the Exchange of Product Model Data) information service provided by the National PDES (Product Data Exchange using STEP) Testbed at the National Institute of Standards and Technology (NIST). All items available through the STEP information service are public domain materials. The Testbed will maintain the on-line system; however, the contributing organizations are responsible for the content and timeliness of the materials provided. The STEP infor-mation service contains both documents and software modules.

PB91-159756 PC A02/MF A01 National Inst. of Standards and Technology, Gaithersburg, MD. National PDES Testbed Mail Server User's Guide.

National PDES Testbed Report Series. S. Ressler. 31 Jan 91, 10p NISTIR-4508

Keywords: \*Electronic mail, Document circulation, Archives, Documents, Access methods, User manuals, \*PDES(Product Data Exchange using STEP), STEP(Standard for the Exchange of Product Model

As part of the Nation PDES Testbed Project, the Information Services Center has established a facility to electronically distribute documents. The facility is based on software known as an 'archive server' or 'mail server'. Electronic documents may be requested and in turn received via electronic mail (e-mail). The report is intended to function both as a user's guide and as a general explanation of the system and its capabilities.

100,952 PB91-167312 PC A04/MF A01 National Inst. of Standards and Technology (TS), Gaithersburg, MD.
NIST Standard Reference Data Products 1991

Catalog.

Special pub. M. W. Chase, and J. C. Sauerwein. Feb 91, 53p NIST/SP-782

Also available from Supt. of Docs. as SN003-003-03063-5. Supersedes PB90-219841.

Keywords: \*Catalogs(Publications), Indexes(Documentation), Chemical analysis, Atomic physics, Reaction kinetics, Properties, Molecular structure, Molecular spectroscopy, Thermochemistry, Thermophysical properties, \*National Institute of Standards and Technology, \*Data bases, Materials science.

The National Institute of Standards and Technology's Standard Reference Data Program provides reliable, well-documented data to scientists and engineers for use in technical problem-solving, research, and development. The catalog lists classic data compilations in hard-copy form and current databases in the Standard Reference Database Series. The edition of the catalog updates many new databases. These data compilations have been subdivided into seven categories. Prices and ordering information are located at the back of the document.

100 953

PB91-189795 Not available NTIS National Bureau of Standards, Gaithersburg, MD. Office of Standards Code and Information. Standardizing Standards.

Final rept.

D. R. Mackay. 1988, 2p Pub. in Visions of the Future, p45-46 1988.

Keywords: \*Standards, Guidelines, Reprints, Standards Engineering Society, Keywords, Titles.

The paper describes the activities of the Standards Engineering Society relating to the development of a draft standard for standards incorporating guidelines for designating standards, selecting titles and key-words for standards, providing abstracts of standards, and establishing formats for different types of standards. A second standard establishing guidelines for the production of catalogs and indexes is described as under development.

100,954

PB92-109016 PC A07/MF A02 National Inst. of Standards and Technology (TS), Gaithersburg, MD. Information Resources and Services Div.

Data Bases Available in the Research Information Center of the National Institute of Standards and

Technology. Special pub. (Final).

D. Cunningham. Sep 91, 131p NIST/SP-818 Supersedes PB91-107284. Also available from Supt. of Docs. as SN003-003-03101-1.

Keywords: \*Data bases, \*Information services, Directories, Indexes(Documentation), Subject indexing, Vendors, Tables(Data), \*NIST.

The publication supersedes and revises NIST SP 799, which is dated September 1990. Data bases are listed by acronyms and by full titles. Citations also include dates covered, brief descriptions, kinds of information each contains, producers, the titles of corresponding hard copy, and vendors. A list of vendors with addresses and telephone numbers precedes the list. The General Subject Index is arranged alphabetically by subject categories and the Cross Reference Index lists variant forms of the names of the data bases in the left column with cross references to the name of the data base used in the publication on the right.

100 955 PB92-126556 PC A03/MF A01 National Inst. of Standards and Technology (CSL),

Gaithersburg, MD. Guide to Schema and Schema Extensibility. Final rept.

K. Rosen, and I. des Fontaines. Nov 91, 35p NIST/SP-500/197

Also available from Supt. of Docs. See also PB90-147919 and PB90-219866. Prepared in cooperation with Geological Survey, Reston, VA. Water Resources

Keywords: \*Information systems, \*Data management, Dictionaries, Data base management, Computer aided software engineering, Information resources manage-

The guide was developed to assist both the casual user of Information Systems (IS) as well as ADP professionals in understanding the concepts behind databases and data dictionary schemas and schema extensibility. It was developed in the context of its application and pertinence to the ANSI standard X3.138-1988, Information Resource Dictionary Systems (IRDS). The guide begins with a set of definitions that

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## Information Systems

provide an understanding of data dictionary and repository terminology. It then follows with a discussion of the IRDS. After establishing these basic definitions, the discussion of schema is initiated. The document also discusses the importance of schema extensibility to the exchange of information between Computer Aided Software Engineering (CASE) tools. Included is a discussion of the CASE tool to IRDS data exchange prototype that was developed at NIST. The document concludes with a discussion of possible future impacts of schema extensibility on the development of standards in areas related to data dictionaries and repositor-

#### Reference Materials

100 956 FIPS PUB 11-3 PC F14 National Inst. of Standards and Technology (CSL),

Gaithersburg, MD.
Guideline: American National Dictionary for Information Systems. Category: Software; Subcatego-

mation Systems. Category: Software; Subcategory: Documentation.
Federal information processing standards (Final).
S. M. Radack. c1991, 150p
Supersedes FIPS PUB 11-2. Also pub. as American Standards Committee, New York rept. no. ANSI-X3.172-1990. Prepared in cooperation with American National Standards Committee, New York.

There is a visual bioter bles visibilities.

Three ring vinyl binder also available: North American Continent price \$7.00; all others write for quote.

Keywords: \*Dictionaries, \*Information systems, National government, Data processing, Computers, \*Federal information processing standards.

The publication adopts ANSI X3.172-1990, AMERICAN NATIONAL DICTIONARY FOR INFORMATION SYSTEMS (ANSDIS), as a FIPS Guideline. The FIPS PUB provides a common reference within the Federal Government for terms and definitions used in the field of information systems including computers, data communications, data processing, text processing, and re-lated fields. The DICTIONARY consists of an alpha-betic listing of terms and their definitions. The DIC-TIONARY includes terms and definitions from the ISO Vocabulary -- Information Systems developed by ISO/ IEC JTC 1/TC 97/SC1: Vocabulary. The revision su-persedes FIPS PUB 11-2 (ANSI X3/TR-1-82) in its en-

100,957

PB91-136507 PC A99/MF A99 National Inst. of Standards and Technology, Gaithers-

National Bureau of Standards Publications 1977-1987. Volume 1. Citations, Key Words, and Abstracts.

Special pub (Final rept. 1977-87).
R. Pardee, E. Gladden, and D. Harris. Aug 90, 1675p
NIST/SP-790-VOL-1

Also available from Supt. of Docs. See also PB91-

Keywords: \*US NBS, \*Bibliographies, Subject index terms, Abstracts, \*National Bureau of Standards, US NIST.

Volume 1 contains full bibliographic citations, key words, and abstracts for 15,746 National Bureau of Standards (NBS) (as of August 23, 1988 the National Institute of Standards and Technology (NIST)) papers published and entered into the National Technical Information Service (NTIS) collection between 1977 and 1987. Also included are several papers published prior to 1977 but not entered into the NTIS collection until 1977. Volume 2 (PB91-136515) contains four indexes to allow the user to identify papers by personal author, key words, title, and NTIS order/report number.

100.958 PC A99/MF A99 PR91-136515 EnviroSystems Supply, Inc., Fort Myers, FL.

National Bureau of Standards Publications 1977-1987. Volume 2. Indexes. Special pub (Final rept. 1977-87). R. Pardee, E. Gladden, and D. Harris. Aug 90, 1442p NIST/SP-790-VOL-2

Also available from Supt. of Docs. See also PB91-

Keywords: \*US NBS, \*Bibliographies, Subject index terms, Indexes(Documentation), Authors, \*National Bureau of Standards, US NIST.

Volume 1 contains full bibliographic citations, key words, and abstracts for 15,746 National Bureau of Standards (NBS) (as of August 23, 1988 the National Institute of Standards and Technology (NIST)) papers published and entered into the National Technical Information Service (NTIS) collection between 1977 and 1987. Also included are several papers published prior to 1977 but not entered into the NTIS collection until 1977. The volume, Volume 2, contains four indexes to allow the user to identify papers by personal author, key words, title, and NTIS order/report number.

PB91-148494 PC A03/MF A01 National Inst. of Standards and Technology, Gaithers-burg, MD. Information Resources and Services Div. Abstract and Index Collection in the Research Information Center of the National Institute of Standards and Technology (Fourth Edition). Special pub. (Final).

D. Cunningham. Dec 90, 36p NIST/SP-803 Also available from Supt. of Docs. as SN003-003-03056-2. Supersedes PB89-103790.

\*Indexes(Documentation), Keywords: \*Abstracts, Technical reports, Information centers, Descriptive cataloging, Subject indexing, \*National Institute of Standards and Technology, \*Technical Information Centers, Research Information Center(NIST).

An alphabetical arrangement of abstracts and indexes available in the Research Information Center (RIC) of the National Institute of Standards and Technology (NIST) is listed by most current title of the publication. Other information includes description of the abstract or index, RIC holdings, principal sources, publisher or association, corresponding RIC data base and the classification number. A general subject and former title/data base name index follow the main text of the

100.960 PB91-171330 PC A12/MF A02 National Inst. of Standards and Technology, Gaithersburg, MD. Office of Information Services. NIST Serial Holdings, 1991. Special pub. (Final)

M. L. Kingston. Feb 91, 268p NIST/SP-777 Also available from Supt. of Docs. as SN003-003-03075-9. Supersedes PB90-183245.

Keywords: \*Periodicals, \*Catalogs(Documentation), \*Collection, \*Information centers, Standards, Libraries, Metrology, \*US National Institute of Standards and Technology, \*NIST.

The publication contains holdings information for approximately 5,000 titles held in the National Institute of Standards and Technology (NIST) Research Information Center, representing current and noncurrent jour-nals, periodicals, annuals, memoirs, proceedings, and transactions

#### General

PB91-189522 Not available NTIS National Inst. of Standards and Technology (NCSL), Gaithersburg, MD. Systems and Software Technology

Document Architecture for Open Systems.

Final rept. R. Hunter, P. Kaijser, and F. Nielsen. 1989, 11p. Pub. in Computer Communications 12, n2 p69-79 Apr

Keywords: \*Documents, \*Standards, Data processing, Information transfer, Format, Reprints, \*ODA(Office Document Architecture), \*Document processing.

The document provides a tutorial overview to the Office Document Architecture (ODA) standard--ISO 8613. The document presents historical information about the development of the standard and summarizes the features of ODA. The prime objective of ODA is to provide for the representation and encoding of documents so that they can be transferred between different document processing systems. ODA documents may be transferred in three forms: formatted form, processable form, and formatted processable These forms are described as well as other concepts of ODA including: logical and layout structures, document constituents, content architectures, and so on. The ODA standard is briefly, yet thoroughly, described.

100,962 PB92-116383 PC A03/MF A01 National Inst. of Standards and Technology, Gaithers-

Guide for the Use of the International System of Units: The Modernized Metric System.

Special pub. (Final).
A. O. McCoubrey. Sep 91, 39p NIST/SP-811
Also available from Supt. of Docs. as SN003-003-03113-5. See also PB92-109032 and N73-26969.

Keywords: \*International system of units, \*Metric system, \*Conversion tables, Units of measurement.

The Guide for the Use of the Modernized Metric System is a practical tool for the use of authors in the preparation of technical manuscripts in conformance with the NIST policy that requires the use of the International System of Units (SI) for all publications. For this purpose, the Guide replaces Exhibit 2-D of Chap-ter 2 in the NBS Communications Manual for Scientific, Technical, and Public Information; it has also been prepared to support the broad objectives of the NIST program for metric conversion. The Guide is further intended to replace NBS Letter Circular LC 1120 (1979) as a document suitable for distribution to other Government agencies and the public.

# MANUFACTURING **TECHNOLOGY**

## Computer Aided Design (CAD)

PB91-147579 Not available NTIS Mational Bureau of Standards (NEL), Gaithersburg, MD. Factory Automation Systems Div.

UNIX in the Government's Automated Manufactur-

ing Research Facility (AMRF).

Final rept.

D. Libes. 1986, 6p Pub. in Government Computer News 5, n6 p1-6, 14 Feb 86.

Keywords: \*UNIX(Operating system), \*Research projects, Computer aided manufacturing, Automation, Computer aided design, Robotics, Computer systems hardware, Programming languages, Operating systems(Computers), Reprints, \*Automated Manufacturing Research Facility.

The report discusses all projects in the Automated Manufacturing Research Facility (AMRF) using UNIX. Brief descriptions of each project include machine, language and version of UNIX used.

100,964 PB91-157164 PC A04/MF A01 National Inst. of Standards and Technology, Gaithersburg, MD.

NIST Express Working Form Programmer's Reference (Revised November 1990). National PDES Testbed Report Series.
S. N. Clark, Dec 90, 52p NISTIR-4407

See also PB90-269531.

Keywords: \*Computer aided design, \*Computer aided manufacturing, \*Standards, \*Software tools, Computer programming, Mathematical models, Programming manuals, Parsers, Translators, \*PDES(Product Data Exchange Specifications), National Institute of Standards and Technology.

The Product Data Exchange Specification (PDES) is an emerging standard for the exchange of product information among various manufacturing applications. PDES includes an information model written in the Ex-

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press language; other PDES-related information models are also written in Express. The National PDES Testbed at the National Institute of Standards and Technology (NIST) has developed software to manipulate and translate Express models. The software consists of an in-memory working form and an associated Express language parser, Fed-X. The internal operation of the Fed-X parser is described. The implementation of the data abstractions which make up the Express Working Form is discussed, and specifications are given for the Working Form access functions. The creation of Express language translators using Fed-X is discussed.

100,965 PB91-167262 PC A03/MF A01 National Inst. of Standards and Technology (NCSL), Gaithersburg, MD. Information Systems Engineering

SQL3 Support for CALS Applications. L. Gallagher. Feb 91, 39p NISTIR-4494

Keywords: \*Computer aided manufacturing, \*Data base management systems, Computer aided design, Federal information processing standards, Standardization, Data processing security, Recursive functions, \*CALS, \*SQL3 database language, ANSI(American National Standards Institute), ISO(International Organization for Standards) nization for Standardization).

Previous reports to CALS have identified the importance of Database Language SQL in CALS Phase II requirements. In particular, a July 1989 point paper on SQL and RDA identified features in the existing SQL standard and its near-term SQL2 replacement that are most appropriate to CALS data management con-cerns. The report focuses on SQL3, a follow-on standardization project for major new SQL enhancements that is expected to be adopted by American National Standards Institute (ANSI), International Organization for Standardization (ISO), and as a Federal Information Processing Standard (FIPS) in the mid 1990's. Many of the proposed SQL3 features are of particular importance to the Standard for the Exchange of Product model data (STEP) because of that standard's unique data modeling and data access requirements. Existing and planned features in SQL3 may not satisfy all STEP requirements, but they should provide an appropriate base from which many requirements can be suitably addressed. Since features in SQL3 are just now being specified, they are open to modification and improve-ment to best suit CALS needs. The report identifies the major enhancements under consideration by the ANSI and ISO SQL standardization committees and relates them to known manufacturing and product manage-ment requirements. It also discusses the status of these features in the SQL3 specification and indicates opportunities available to CALS to influence further development.

100.966 PB91-184788 PC A03/MF A01 National Inst. of Standards and Technology (BFRL),

Gaithersburg, MD.
STEP: Standard for the Exchange of Product Model Data Resource Integration: Semantic and

Syntactic Rules.
W. F. Danner, D. T. Sanford, and Y. Yang. Mar 91, 21p NISTIR-4528

Keywords: \*Standards, \*Models, Computer aided design, Semantics, Syntax, \*STEP(Standard for the Exchange of Product Model Data), PDES(Product Data Exchange using STEP), National Institute of Standards and Technology.

The report documents the rules that are used in the integration of Standard for the Exchange of Product Model Data (STEP) draft resource models. The rules are applied in the development of the STEP Integrated Resource that satisfies application requirements for

PB91-216663 PC A03/MF A01 National Bureau of Standards (NEL), Gaithersburg, MD. Machine Intelligence Group. Apparel STEP Translator.

H. T. Moncarz, and Y. T. Lee. Jun 91, 19p NISTIR-4612

Sponsored by Defense Logistics Agency, Alexandria,

\*Computer aided Keywords: \*Clothing industry, design, Computer aided manufacturing, Prototypes, Data structures, File structures, Format, Translators, Man computer interface, Models, Standardization, \*STEP(Standard for the Exchange of Product Model Data), National Institute of Standards and Technology.

The paper describes the implementation of a proto-type computer program for translating apparel pattern data between different file storage formats. The program demonstrates the feasibility of using a single, standard format as a mechanism for exchanging data between dissimilar pattern design systems. The software was developed as part of an ongoing project to incorporate apparel applications into the Standard for the Exchange of Product Model Data (STEP), an emerging international standard. In the short term, the project goal is to develop a neutral data format for exchanging two-dimensional pattern data between apparel computer aided design (CAD) systems. In the longer term, the goal is to develop an information model that can be used to encompass the entire apparel life cycle. This achievement would allow all of the processes involved in the apparel life cycle to share the same data.

100,968

PB91-222620 PC A03/MF A01 National Inst. of Standards and Technology, Gaithersburg, MD.

Configuration Management of the STEP Documents: Procedures and System Requirements. National PDES Testbed Report Series.

S. B. Katz. 10 Jul 91, 20p NISTIR-4629 Sponsored by Assistant Secretary of Defense (Production and Logistics), Washington, DC. Computer-Aided Acquisition and Logistic Support Program.

Keywords: \*Computer aided manufacturing, \*Standards, \*Product development, Computer aided design, \*STEP(Standard for the Exchange of Product Model Data), ISO(International Organization for Standardization), PDES(Product Data Exchange using STEP), National Institute of Standards and Technology, Configuration management.

The paper proposes configuration management procedures that support the International Organization for Standardization's (ISO's) approval process for the Standard for the Exchange of Product Model Data (STEP), and introduces requirements for incorporating those procedures into a configuration management system.

100,969

PB92-112374 PC A04/MF A01 National Inst. of Standards and Technology, Gaithersbura, MD.

Proposed Testing Methodology for STEP Applica-tion Protocol Validation. National PDES Testbed Report Series.
M. J. Mitchell. 26 Sep 91, 51p NISTIR-4684

Sponsored by Assistant Secretary of Defense (Production and Logistics), Washington, DC. Computer-Aided Acquisition and Logistic Support Program.

Keywords: \*Protocols, \*Tests, \*Product development, \*Standards, Computer aided design, Computer aided manufacturing, Standardization, Specifications, manufacturing, Standardization, Specifications, Models, Methodology, \*STEP(Standard for the Exchange of Product Model Data), PDES(Product Data Exchange Using STEP).

An Application Protocol (AP) is a specification for a subset of the data described by the Standard for the Exchange of Product Model Data (STEP). Application Protocols are designed to permit practical implementations of STEP. Validation is needed to ensure that the technical solutions provided by the AP will work in a practical sense. The document proposes that the STEP development policy be strengthened to require that Application Protocols be validated prior to being submitted for standardization. Justification for the additional requirement on Application Protocols is provided. The body of the paper describes a series of validation techniques that are apropriate for the develop-ment methods used by STEP. A process is proposed under which these validation techniques should be applied. In addition, the paper describes the contribution that AP validation could make to conformance testing.

100.970

PB92-112523 PC A04/MF A01 National Inst. of Standards and Technology, Gaithersburg, MD.

Test Plan for Validating a Context Driven Integrated Model (CDIM) for Sheet Metal Die Design. National PDES Testbed Report Series.

K. K. Jurrens. Aug 91, 55p NISTIR-4699 Sponsored by Assistant Secretary of Defense (Production and Logistics), Washington, DC. Computer-Aided Acquisition and Logistic Support Program.

Keywords: \*Computer aided design, \*Computer aided manufacturing, \*Models, \*Metal sheets, \*Dies, Prodmanufacturing, Models, Metal and Scot, Protocols, Software tools, Facilities, Training, Scheduling, CDIM/Context Driven Integrated Model), PDES(Product Data Exchange Using STEP), STEP(Standard for the Exchange of Product Model Data).

The document defines the Test Plan that will govern testing of the first Context Driven Integrated Model (CDIM) developed by the PDES, Inc. Sheet Metal Project (CDIM SM1). The Test Plan specifies the test objectives, methodology, constraints, requirements, and the state of the evaluation criteria, resources, deliverables, and issue procedures for the testing activity. In addition, the document provides a brief introductory overview of CDIM

100,971 PB92-123090 PC A06/MF A02 National Inst. of Standards and Technology, Gaithersburg, MD.

Validation Testing Laboratory User's Guide. National PDES Testbed Report Series.

N. Breese, M. McLay, and G. Silvernale. Sep 91, 105p NISTIR-4683

See also PB91-107581. Sponsored by Assistant Secretary of Defense (Production and Logistics), Washington, DC. Computer-Aided Acquisition and Logistic Support Program.

Keywords: \*Computer aided design, \*Computer aided manufacturing, \*Standardization, \*Product development, Standards, Data processing, UNIX(Operating system), Utility routines, Computer vision, Translator routines, Compilers, Parsers, Editing routines, Data base management systems, User manuals(Computer programs), Computer systems hardware, Computer systems programs, PDES(Product Data Exchange using STEP), STEP(Standard for The Exchange of Product model data), CALS, US NIST.

Product Data Exchange Using STEP (PDES) is the United States activity supporting the Standard for the Exchange of Product Model Data (STEP), a proposed international standard for product data representation and exchange. The document is a quick reference for those using the Validation Testing Laboratory of the National PDES Testbed. It is not intended for those wishing to learn about the tools in the Testbed but is rather for those who already have a working knowledge of the programs and terminology. The Testbed was initiated in 1988 under the sponsorship of the U.S. Department of Defense Computer-aided Acquisition and Logistic Support (CALS) program. A major goal of the Testbed is to provide technical leadership in a national effort to implement a complete and useful specification for the exchange of product data. The specification must be designed to meet the needs of U.S. industry and the CALS program. The National PDES Testbed supports and actively participates in the international effort to develop (STEP).

#### Computer Aided Manufacturing (CAM)

100.972 PB91-132142 PC A03/MF A01 National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Factory Automation Systems Div. Software and Computer Integrated Manufacturing. H. M. Bloom. Nov 90, 11p NISTIR-4468

Keywords: \*Computer aided manufacturing, \*Computer software, Systems engineering, Production management, Data management, Communications management, Standards, Data bases,

The paper outlines present and future directions for software in a Computer Integrated Manufacturing (CIM) environment. The three major CIM components production management, data management, and communications management -- are described in

## Computer Aided Manufacturing (CAM)

terms of software available today and future software based on emerging international standards. Key stand-ards efforts such as product data exchange, open sys-tems interfaces, database systems frameworks, and CIM frameworks are described.

100,973 PB91-134718 Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Center for Mfg. Engineering.
Al in Manufacturing: The NBS AMRF as an Intelligent Machine. Final rept.

Pinal rept.
D. A. Swyt. 1988, 16p
Pub. in Proceedings of International Conference on Expert Systems and the Leading Edge in Production Planning and Control, Intelligent Manufacturing (1st), p357-372 1988.

Keywords: \*Artificial intelligence, Robots, Standards, Automation, Reprints, \*Automated Manufacturing Research Facility, \*Computer aided manufacturing, National Institute of Standards and Technology, Control systems, Knowledge representation.

Consisting of robots, machine tools and computers, the Automated Manufacturing Research Facility (AMRF) is being integrated using a real-time, sensory-feedback, data-driven hierarchical control architecture. As such, the AMRF is a research tool for investigating the manufacturing enterprise as a system of in-telligent machines. The report describes the AMRF in terms of its real-time control system architecture; notes the role of symbolic languages, knowledge-rep-resentation, sensory-processing and other aspects of artificial intelligence (AI) in its development; and speculates on further application of AI in future intelligent manufacturing systems similar in form to the AMRF.

100,974 PB91-14**7**59**5** PB91-147595 Not available NTIS National Bureau of Standards (ICST), Gaithersburg, MD. Systems and Network Architecture Div. Application of OSI Protocols for Plant Information Networks.

Final rept.

R. J. Linn. 1987, 21p Pub. in Proceedings of International Conference on Foundations of Computer Aided Process Operations, Park City, UT., July 5-10, 1987, p453-473.

Keywords: \*Computer aided manufacturing, \*Communication networks, \*Protocols, Standards, Computer networks, Information systems, Computer architecture, Reprints, OSI(Open Systems Interconnection), MAP(Manufacturing Automation Protocol), GOSIP(Government Open Systems Interconnection Profile), TOP(Technical and Office Protocols).

The International Organization for Standardization (ISO) has developed a set of standards defining data communications protocols for heterogeneous computer systems. Collectively, these protocols are called the Open Systems Interconnection (OSI) protocols. Computer and communications equipment manufacturers are beginning to provide implementations of these products of the provide implementations of the pro tocols as product offerings which can be applied to manufacturing plant information networks. Summaries are provided of the functional aspects of selected international standards, and their relationships to U.S. Government and industrial profiles of the same standards. These profiles are the Government Open Sysards. These profiles are the Government Open Sys-tems Interconnection Profile (GOSIP), Manufacturing Automation Protocol (MAP) and Technical and Office Protocols (TOP). The MAP profile was developed under the leadership of General Motors Corporation with the objective of applying emerging international standards to plant information networks in highly auto-mated factories. The TOP and GOSIP profiles extend the application of the same kernel of protocols to scithe application of the same kernel of protocols to sci-entific, engineering, and office environments which may be geographically or locally distributed. Applica-tion of OSI protocols for plant information networks is illustrated by example.

100,975 PB91-148122 PB91-148122 Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Center for Mfg. Engineering.
CIM, Data and Standardization within the NBS Final rept. D. A. Swyt. 1988, 7p Pub. in Robotics 4, n2 p193-199 Jun 88.

Keywords: \*Computer aided manufacturing, \*Data management, \*Standards, Automation, Robotics,

Computer aided design, Reprints, Automated Manufacturing Research Facility, National Institute of Standards and Technology

Computer-Integrated-Manufacturing (CIM) is key to the factory of the future, shared data is key to integration, and interface standards are key to data-sharing. Within its Automated Manufacturing Research Facility (AMRF), the U.S. National Bureau of Standards is addressing issues of standardized interfaces in the four principal data activities of the automated factory: data preparation, data administration, data communication, and data-driven control. By means of such interface standards, the flexibly-automated, robotics-based, computer-integrated factory of the future can be realized in a modular, easily-integratable, multi-vendor form.

100,976 PB91-148130 PB91-148130 Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Center for Mfg. Engineering.
Innovation in Manufacturing Technology: A View from NBS. Final rept.
D. A. Swyt. 1985, 16p
Pub. in Proceedings of Conference on Manufacturing

Research: Organizational and Institutional Issues, Stuttgart, West Germany, August 19-23, 1985, p1-16.

Keywords: \*Computer aided manufacturing, \*Manufacturing, \*Technology assessment, Automation, Process control, Robotics, Automatic control, Man machine systems, Standardization, Industrial plants, Industries, Reprints.

Based on work in measurements and standards for the automated manufacturing of discrete parts, the view of manufacturing technologies from the National Bureau of Standards is one of substantial change and growth following the current seminal stage of development. Economics and the desire for advanced capabilities drive the change. Relative to technological ideas being developed in laboratories such as NBS, current industrial robots are crude and the most automated processes not under adequate control. Simple extrapolation of current work will result in profoundly more advanced robotic systems and effective automated control of entire factories. This impending change provides substantial challenges for coordinated research in three key areas: the basics of unit processes, control systems for intelligent machines, and the integration of unit processes and intelligent machines into whole factory systems.

PB91-167320 PC A03/MF A01 National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Factory Automation Systems Div. Engineering Design Laboratory Guide.
A. B. Feeney. 19 Feb 91, 19p NISTIR-4519

Keywords: \*Computer aided manufacturing, \*Computer aided design, Structural analysis, Finite element analysis, Knowledge base, Computerized simulation, Numerical control, Clothing, US NIST, \*Engineering Design Laboratory, \*Factory automation, Geometric medeling.

The document provides a brief description of the systems available for use in the Engineering Design Laboratory at the National Institute of Standards and Technology, Gaithersburg, Maryland. The Engineering Design Laboratory was established to study the process of design, how design information can be represented, and how to make design information available to necessary systems throughout a product's life cycle. The document also discusses opportunities for collaborative or independant research in the Engineering Design Lab.

100,978 PB91-167700 PB91-167700 PC A04/MF A01 National Inst. of Standards and Technology (CAML), National Inst. of Standards and Technology (CAML), Gaithersburg, MD. Office of Applied Economics. Automan 2.0: Decision Support Software for Automated Manufacturing Investments. User Manual. S. F. Weber. Mar 91, 75p NISTIR-4543, NIST/SW/DK-91/007A, NIST/SW/DK-91/009A For system on diskette, see PB91-506568 and PB91-507194.

Keywords: \*Computer aided manufacturing, \*Investments, \*Decision support sysems, Automation, Life cycle costs, Present worth, Evaluation, Comparison, Ranking, Ratings, User manuals(Computer programs), Documentation, Automan computer program.

The manual documents Automan, a microcomputer program designed to support multi-criteria decisions about automated manufacturing investments. The program permits users to combine quantitative and qualitative criteria in evaluating investment alternatives. Quantitative criteria could include such traditional financial measures as Life-Cycle Cost and Net Present Value as well as such engineering performance measures as throughput and setup time. Qualitative criteria could include flexibility and product quality. First, the user specifies the evaluation criteria and the investment alternatives to be evaluated. Second, the user makes pairwise comparisons between criteria to establish their weights. Third, the user rates each investment alternative with respect to the criteria. The pairwise comparison process helps the user rate the qualitative criteria, while measured performance data, such as cost, setup time, or throughput, can be entered for quantitative criteria. Automan combines ratings with criteria weights into an overall rating for each invest-ment alternative and then ranks alternatives. Finally, graphical sensitivity analysis can be conducted to visu-alize the overall ratings of every alternative for every possible weight that could be assigned to any criterion. Automan comes with sample decision models and a manual that includes a detailed tutorial, a glossary of evaluation criteria, a bibliography, and an index.

100,979 PB91-174623 Not available NTIS
National Inst. of Standards and Technology (NEL),
Gaithersburg, MD. Precision Engineering Div.
High Precision Gaging with Computer Vision Systems tems. Final rept.

T. D. Doiron. 1990, 12p Contract DE-Al05-85OR21584 Sponsored by Department of Energy, Oak Ridge, TN. Pub. in Industrial Metrology 1, p43-54 1990.

Keywords: \*Computer vision, Edge detection, Video equipment, Interfaces, Cameras, Precision, Accuracy, Reprints, \*Gaging, Robot vision.

In order to use a computer vision system for high accuracy gaging, the intensity array reported to the computer from the camera must correspond closely to the geometry of the part to be measured. To verify this correspondence for two different vision systems, a number of tests are reported and discussed. A number of effects due to the camera sensor geometry, the type of edge finder employed, the thermal properties of the camera, and the interface method used between the camera and computer are explored.

100,980 Not available NTIS PB91-174938 PB91-174938
National Bureau of Standards (NEL), Gaithersburg, MD. Factory Automation Systems Div.
Error Prevention and Detection in Data Preparation for a Numerically Controlled Milling Machine.

Final rept.

T. R. Kramer, and W. T. Strayer. 1987, 19p Grant 70NANB4H0006

Sponsored by Catholic Univ. of America, Washington,

Pub. in Proceedings of Symposium on Intelligent and Integrated Manufacturing Analysis and Synthesis, Boston, MA., December 13-18, 1987, p195-213.

Keywords: \*Computer aided manufacturing, \*Error detection codes, \*Milling machines, Numerical control, Workstations, Detection, Software(Computers), Errors, Checking(Proving), Milling(Machining), Quality control, Reprints.

In the Vertical Workstation (VWS) of the NBS Automated Manufacturing Research Facility, metal parts are machined automatically from a feature-based design. A simple two-and-a-half dimensional part may be designed and machined within an hour, allowing half the time for design input. Workstation activity may be divided into design, process planning, data execution, and physical execution stages. In order to make VWS operation safe and accurate, extensive error prevention and detection (verification) procedures have been incorporated in the data preparation stages, particularly design and data execution. The software for these stages is about 700 pages of LISP code and runs on a Sun computer. About a quarter of the code is solely for error prevention. Automatic verification includes, design editor dialogs, design enhancement, design verification (subdivided into parameter type checks, feature verification, and reference feature fit checking), process plan verification, workpiece verification,

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part model checking, and other items. Interactive verification includes design drawing, workpiece model drawing, and tool path drawing. The feature verifiers are prepared by a rule-based automatic programming subsystem.

100,981 PB91-175091 Not available NTIS Mational Bureau of Standards (NEL), Gaithersburg, MD. Center for Mfg. Engineering.
U.S. Manufacturing Systems: Factories Past,

Present, and Future.

Final rept.
D. A. Swyt. 1987, 13p
Pub. in Proceedings of U.S./Japan Conference on Passing Research Perspectives, Tokyo, Japan, Manufacturing Research Perspectives, Tokyo, Japan, October 27-29, 1986, p38-50 1987.

Keywords: \*Computer aided manufacturing, \*Robots, Automation, United States, Competition, Industrial plants, Robotics, Reprints, Automated Manufacturing Research Facility.

U.S. manufacturing is in the throes of a fundamental changeover in its production technologies and systems. Under pressures of rapid globalization of its own markets, fierce competition from technologically-capable trading partners, and an aging industrial base, the United States is beginning to move from the labor-intensive mass production factory of the past to the information-intensive, custom-quantity factory of the future. The principle technology of the factory of the future is robotic-based, computer-integrated, flexible automation. In machine-tool-based factory production, the computer and robot have been joined with the machine-tool-based factory production. chine tool to form the flexible manufacturing cell, the first realization on the shop floor of the central principles of the factory of the future. To allow achievement of the total factory of the future, manufacturing re-search in the United States, represented by work at the Automated Manufacturing Research Facility, is di-rected at bringing the entire factory under computer-integrated control.

100,982 PB91-193367 PC A05/MF A01 National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Factory Automation Systems Div. Concurrent Engineering through Product Data Standards.

G. P. Carver, and H. M. Bloom. May 91, 77p NISTIR-4573

Keywords: \*Computer aided manufacturing, \*Standards, Concurrent processing, Automation, Information processing, Data bases, Computer aided design, \*Concurrent engineering, STEP(Standard for the Exchange of Product Model Data), PDES(Product Data Exchange using STEP), National Institute of Standards and Technology. and Technology.

Concurrent engineering involves the integration of people, systems and information into a responsive, efficient system. Integration of computerized systems allows additional benefits: automatic knowledge capture during development and lifetime management of a ture during development and lifetime management of a product, and automatic exchange of that knowledge among different computer systems. Critical enablers are product data standards and enterprise integration frameworks. A pioneering assault on the complex technical challenges is associated with the emerging international Standard for the Exchange of Product Model Data (STEP). Surpassing in scope previous standards efforts, the goal is a complete, unambiguous, computer-readable definition of the physical and functional characteristics of a product throughout its life cycle. U.S. government agencies, industrial firms, and standards organizations are cooperating in a pro-Inte cycle. U.S. government agencies, industrial firms, and standards organizations are cooperating in a program, Product Data Exchange using STEP (PDES), to develop and implement STEP in a shared-database environment. PDES will lead to higher, integrated levels of automation based upon information standards and frameworks. U.S. manufacturers will benefit from concurrent engineering without sacrificing the historical strengths and traditions of individuality, initiative and intellectual property rights. Concurrent engineering nistorical strengths and traditions of individuality, initiative, and intellectual property rights. Concurrent engineering, through information technology and standards, represents the power of a new industrial revolution. The role of the National Institute of Standards and Technology (NIST) National PDES Testbed, technical leadership and a testing-based foundation for the development of a STEP, is described.

100,983 PB91-194449

PC A04/MF A01

National Inst. of Standards and Technology, Gaithersburg, MD.

Extracting STEP Geometry and Topology from a Solid Modeler: Parasolid-to-STEP.
T. R. Kramer. 2 May 91, 56p NISTIR-4577

Prepared in cooperation with Catholic Univ. of America, Washington, DC. Sponsored by Assistant Secretary of Defense (Production and Logistics), Washington, DC. Computer-Aided Acquisition and Logistic Support Program.

Keywords: \*Solids, \*Three dimensional models, \*Translators, Mathematical models, Computer soft-ware, Translator routines, Topology, Geometry, \*STEP(Standard for the Exchange of Product Model Data), \*Parasolid software system.

Parasolid is a commercial solid modeling software system. It uses a manifold boundary representation. STEP is an emerging international Standard for the Exchange of Product Model Data. Included in STEP are proposed standards for Topology and Geometry (which provide the definitions of data types required for building boundary representations) and for physical files representing products. Parasolid-to-STEP is a software system written in the C programming language for translating a Parasolid format boundary repgrade to translating a Parasonal format boundary representation file giving the shape of an object into a STEP format file describing the same shape. The system handles elementary curves (lines, circle, ellipse) and surfaces (plane, sphere, cylinder, cone, torus).

100.984 PB91-194480 PC A03/MF A01 National Inst. of Standards and Technology, Gaithersburg, MD.
Configuration Management Concepts Document.

National PDES Testbed Report Series. S. B. Katz. 26 Apr 91, 33p NISTIR-4538

\*File management systems, \*Access, Computer aided manufacturing, Documents, Software engineering, Quality assurance, \*CMS(Configuration Management System), \*STEP(Standard for the Exchange of Product Model Data), ISO(International Organization for Standard ganization for Standardization).

The purpose of the document is to establish Configuration Management (CM) concepts to be applied in support of the development of the Standard for the Exchange of Product Model Data (STEP). Configuration management is the management of change. It is a formal discipline which provides methods and tools to: identify components, versions and baselines of select-ed items; and control changes to those items. CM provides a method for logically grouping related components throughout the various stages of product development. It also provides visibility and traceability for the evolving status of each item. An effective CM system thus identifies, controls, records, and reports on any functional, physical or status changes to the controlled items.

PB91-195172 Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Robot Systems Div.

CAD Directed Robotic Deburring.

Final rept.

K. N. Murphy, R. J. Norcross, and F. M. Proctor.

1988, 7p
Pub. in Proceedings of International Symposium on Robotics and Manufacturing (2nd): Research, Education, and Applications, Albuquerque, NM., November 16-18, 1988, p959-965.

Keywords: \*Robots, \*Deburring, \*Computer aided manufacturing, \*Computer aided design, Robotics, Real time systems, Off line systems, Programming, Control systems, Paths, Automation, Interactive graphics, Algorithms, Data structures, Reprints, Automated Manufacturing Research Facility.

At the Automated Manufacturing Research Facility, re-At the Automated Manufacturing Hesearch Facility, research is being conducted on techniques to automate robot programming. A technique has been developed and demonstrated in the Cleaning and Deburring Workstation which uses Computer Aided Design (CAD) geometry data to automatically generate robot deburring paths. Using a graphics interface, an operator specifies the edges on a part to be deburred, the deburring tools to be used, and the speeds, feed rates, and contact forces desired. Deburring paths are generated and sent to a PLIMA 760 robot controlled by the ated and sent to a PUMA 760 robot controlled by the Real-Time Control System. The robot uses a two-pass

technique for deburring. On the first pass, the robot uses force feedback to correct the deburring path points to account for robot kinematic errors, tool wear, and minor part misplacement. On the second pass, the robot follows the corrected path, deburring the part. The paper describes the techniques, algorithms and data formats used in the robotic deburring system.

100.986

PB91-195495 Not available NTIS
National Inst. of Standards and Technology (NEL),
Gaithershura MD Belef Surface Standards Gaithersburg, MD. Robot Systems Div. Automating Robot Programming in the Cleaning and Deburring Workstation of the AMRF.

Final rept.

F. M. Proctor, K. N. Murphy, and R. J. Norcross.

1989, 11p Pub. in Proceedings of SME Conference Deburring and Surface Conditioning '89, San Diego, CA., February 13-16, 1989, p1-11.

Keywords: \*Robots, \*Automation, \*Workstations, \*Computer aided manufacturing, Robotics, Scheduling, Materials handling, Deburring, Cleaning, Precision finishing, Buffing, Process control, Reprints, Automated Manufacturing Research Facility.

In the cleaning and deburring workstation, two robots cooperate to accomplish deburring, buffing, cleaning, and handling of machined parts. A technique has been developed which uses part geometry data to automati-cally generate robot paths. Using a graphics interface, an operator specifies how a part is to be gripped, fix-tured, deburred, buffed, and cleaned. A path planner combines the process plan with geometry data to compute robot paths. A workstation controller coordinates the actions of both robots, allowing various steps in the finishing process to be performed simultaneously. The paper describes the methods used to automate the finishing process.

100.987

Not available NTIS
National Inst. of Standards and Technology (NEL),
Gaithersburg, MD. Center for Mfg. Engineering.
Issues in the Design and Implementation of a
System Architecture for Computer Integrated
Manufacturing.
Final rept

Final rept. Pub. in International Jnl. of Computer Integrated Manufacturing 2, n2 p65-76 Mar/Apr 89.

Keywords: \*Computer aided manufacturing, \*Systems engineering, \*Computer architecture, Production planning, Production control, Data management, Automation, Computer systems hardware, Computer systems programs, Reprints.

The advent of sophisticated automation equipment and computer hardware and software is changing the way manufacturing is carried out. To be competitive, manufacturing companies must integrate these new manufacturing companies must integrate these new technologies into their existing and future factories. In addition, they must integrate the planning, control, and data management methodologies needed to make effective use of those technologies. The paper discusses several issues related to the design and implementation of a system architecture which can serve as the basis for those integration efforts. That architecture includes separate architecture for production ture includes separate architecture for production planning and control, data management, and data communications.

100,988

PB91-203356 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Factory Automation Systems Div. Parser That Converts a Boundary Representation into a Features Representation.

Final rept.

T. R. Kramer. 1989, 10p Contract NANB-7-H0716 See also PB89-160634. Sponsored by Catholic Univ. of America, Washington, DC.

Pub. in International Jnl. of Computer Integrated Manufacturing 2, n3 p154-163 May/Jun 89.

Keywords: \*Computer aided manufacturing, \*Machining, \*Parsers, Workstations, File structures, Feature extraction, Computer aided design, Pattern recognition, Boundaries, Reprints, VWS2 computer program, Automated Manufacturing Research

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## Computer Aided Manufacturing (CAM)

PDES(Product Data Exchange Specification), STEP(Standard for The Exchange of Product Data).

The VWS2 B-rep Parser is a computer program written The VWS2 B-rep Parser is a computer program written in LISP that takes a file giving the boundary representation of a part as input and produces a file giving a feature-based representation of the part as output. The format of the input file is a Product Data Exchange Specification (PDES)/Standard for The Exchange of Product Data (STEP) boundary representation, and the format of the output file is that required by the VMS2 system of the National Institute of Standards VWS2 system of the National Institute of Standards and Technology (NIST) Automated Manufacturing Research Facility (AMRF). The parser deals with a limited range of two-and-a-half dimensional parts. The generrange of two-and-a-half dimensional parts. The general approach to parsing is to expect that the part is parsable and look for arrangements of faces which are the signatures of features. The initial implementation of the approach recognizes five feature types. The approach is extendible to a wider range of feature and subfeature types, and to parts which have features made from several sides. Parts having features which intersect in a complex manner are likely to test the limits of the approach, or be beyond the limits. With the addition of the parser, the AMRF Vertical Workstation is canable of making a part from a PDES/STEP file is capable of making a part from a PDES/STEP file without human intervention.

100,989 PB91-203737 Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Robot Systems Div.

Control Structure for Multi-Tasking Workstations.

Final rept. R. J. Norcross. 1988, 3p

Pub. in Proceedings of IEEE (Institute of Electrical and Electronics Engineers) International Conference on Robotics and Automation, Philadelphia, PA., April 24-29, 1988, p1133-1135.

Keywords: \*Workstations, \*Control systems, \*Manufacturing, Operating systems(Computers), Concurrent processing, Resource allocation, Multiprocessing, Re-

Manufacturing control modules, which are based on hierarchical control theory, decompose commands from a supervisory controller into elementary tasks to be performed by subordinate systems. The ability to simultaneously manage coordinated and independent functions of subordinates, while also processing new commands from the supervisory controller, is benefi-cial in advanced implementations of the controllers. The paper describes a control structure, based on computer operating system principles, which provides the desired capabilities. Utilizing concurrent processing and coordinating tasks via resource allocation provides extensive modularity which simplifies integration, gives a multi-processing environment, and produces the aforementioned capabilities.

100,990 PB91-222596 PC A03/MF A01 National Inst. of Standards and Technology, Gaithers-

Development Plan: Application Protocols for Mechanical Parts Production. National PDES Testbed Report Series.

C. Stark, and M. Mitchell. 2 Jul 91, 36p NISTIR-4628 Sponsored by Assistant Secretary of Defense (Production and Logistics), Washington, DC. Computer-Aided Acquisition and Logistic Support Program.

Keywords: \*Computer aided manufacturing, \*Mechanical devices, \*Protocols, Computer applications, Production planning, Standards, \*STEP(Standard for the Exchange of Product Model Data), PDES(Product Data Exchange using STEP), National Institute of Standards and Technology.

The Standard for the Exchange of Product Model Data (STEP) is being developed as an international standard. The National Product Data Exchange using STEP (PDES) Testbed was established at the National Institute of Standards and Technology (NIST) specifically to address the development and testing of STEP, and to serve U.S. industry in its use of the standard. An Application Protocol (AP) is a specification for a subset of STEP data that can be implemented in an applica-tion system. The APs for Mechanical Parts Production effort will produce an early example of APs being used together in an operational prototype. This effort will develop, fully test, validate, and deliver a set of APs to the STEP Production Cell application systems which support the following: detailed design, process planning, and numerical control programming. The document describes the plan for developing and validating a series of three APs required as input to the STEP Production Cell. The resultant candidate APs, that will be submitted to the International Organization for Standardization (ISO) for inclusion in the standard, will have been validated and thoroughly tested prior to their submission.

100.991

PB91-240796 PC A03/MF A01 National Inst. of Standards and Technology (MEL), Gaithersburg, MD.

Manufacturing Systems Integration Control Entity

Interface Document.
M. K. Senehi, S. Wallace, E. Barkmeyer, S. Ray, and E. K. Wallace. Jun 91, 47p NISTIR-4626

Keywords: \*Computer aided manufacturing, \*Control systems, \*Interfaces, Automation, Hierarchies, Integrated systems, Production planning, Production control, Systems engineering, Models, NIST(National Institute of Standards and Technology), MSI(Manufacturing Systems Integration).

The document defines a set of interfaces for controllers to be incorporated into an integrated manufacturing production planning and control environment that conforms to the National Institute of Standards and Technology (NIST) Manufacturing Systems Integration (MSI) architectural model.

100,992

PB92-108885 PC A03/MF A01 National Inst. of Standards and Technology (MEL), Gaithersburg, MD. Clock for the Manufacturing Systems Integration Testbed.

D. Libes. 5 Sep 91, 19p NISTIR-4666

Keywords: \*Computer aided manufacturing, \*Clocks, \*Computer systems programs, Timing devices, UNIX(Operating system), Scheduling, Automation, Man computer interface, Time, MSI(Manufacturing Systems Integration).

The paper describes a software module that provides timing services to the Manufacturing Systems Integra-tion (MSI) Testbed in the automated factory. The soft-ware 'alarm clock' provides services to other MSI software including: synchrony; real-time, or nonreal-time adjusted in a variety of ways; and alarms at relative or absolute intervals. By providing a central time service, these services are provided more reliably, efficiently, and flexibly than could any client on its own. The paper describes the implementation, interfaces, and how to design and write programs that use it.

PC A03/MF A01 PB92-112234 National Inst. of Standards and Technology, Gaithers-

Conceptual Architecture for a Mechanical Parts
Production System Based on STEP. National PDES
Testbed Rept. Series.

E. J. Barkmeyer, J. E. Fowler, and S. P. Magleby. 27 Sep 91, 39p NISTIR-4685

Prepared in cooperation with Brigham Young Univ., Provo, UT.

Keywords: \*Computer aided manufacturing, \*Mechanical devices, \*Standards, \*Data processing, Computer aided design, File management systems, Protocols, Production models, Systems design, Data bases, Computer systems programs, Product development, \*STEP(Standard for the Exchange of Product Model Data), PDES(Product Data Exchange Using STEP)

The Standard for the Exchange of Product Model Data (STEP) is an emerging standard addressing the prob-lems of data exchange and representation of pro-duced goods in a variety of manufacturing enterprises. Given that the initial STEP specifications largely pertain to mechanical parts production, this domain is an appropriate context for intial STEP implementations. The document describes an architecture for systems realizing a mechanical parts production capability using STEP data exchange. The functions of the major systems and relationships between systems is discussed. Software components which could be used to implement major systems are identified. Major emphasis is given as to how STEP is implemented and used in the context of the architeture.

100,994 PB92-112242

PC A04/MF A01

National Inst. of Standards and Technology (MEL), Gaithersburg, MD.

Manufacturing Systems Integration: Initial Architecture Document.

M. K. Senehi, E. Barkmeyer, M. Luce, S. Ray, E. K. Wallace, and S. Wallace. Sep 91, 70p NISTIR-4682 See also PB91-240796. Sponsored by Naval Research Lab., Washington, DC. Navy Manufacturing Technology Program.

Keywords: \*Computer aided manufacturing, \*Systems engineering, \*Production planning, \*Production control, Computer architecture, Systems design, Automation, Industrial plants, Hierarchies, Models, Error correction codes, Process control, Control systems, Data processing, Man computer interface, Materials handling, Data management, Resource allocation, Production management.

The goal of the Manufacturing Systems Integration (MSI) project at the National Institute of Standards and Technology (NIST) is to develop an approach to solving the problem of incompatible data and control procine esses within a manufacturing enterprise. A major activity of the MSI project is the development of a system architecture that incorporates an integrated production planning and control environment. A particular difficulplanning and control environment. A particular difficulty in developing such an architecture is the sharing of
information between engineering, production management and control systems; there are no standards
specifying the interactions among such systems. The
MSI team is developing a testbed environment which
allows experimentation with integrated production
management and control systems. A critical feature of
the testbed is the specification of an architecture and
interfaces which allow the incorporation of commercial products and university-built prototype systems that support production engineering and control. The vali-dation of the architecture will be via a demonstration of the production of selected parts, using either actual or emulated shop floor equipment or any combination of both. The document describes the first draft of that ar-chitecture and serves as an interim report to record progress in the architecture design.

100,995

PB92-112572 PC A05/MF A01 National Inst. of Standards and Technology (MSEL),

Gaithersburg, MD.
Intelligent Processing of Materials, Technical Activities 1991. (NAS-NRC Assessment Panel, November 14-15, 1991).

Annual rept. H. T. Yolken, 1991, 96p NISTIR-4693 See also PB89-151823 and PB91-143339.

Keywords: \*Artificial intelligence, \*Process control, \*Materials, \*Nondestructive tests, Magnetic properties, Steels, Feasibility analysis, Expert systems, Thermomechanical treatments, Metals, Powder metallurgy, Aluminum, Ceramics, Polymers, Detectors, On-line systems, Standards, US NIST.

Contents: Intelligent Processing of Rapidly solidified metal powders by inert gas atomization; Progress Towards Development of an Intelligent Processing System for On-line Control of Steel Sheet Formability; Thermomechanical Processing of Steels; Magnetic Methods for Evaluation of Mechanical Properties of Steels; Ultrasonic Sensing of Liquid/Solid Interfaces in Metals; Physical and Mechanical Metallurgy and Sensor Technology Development for Intelligent Processing of Soldered Assemblies; Temperature Measurement in Aluminum Processing; Fluorescence and Optical Monitoring of Polymer Processing; Coatings Technology Consortium; Measurement of Dispersion of Ceramic Powders in Dense Slurries Using Electroacoustics; Application of NMR Imaging Technique for Intelligent Processing of Materials; Eddy Current Sensing of Carbon-Carbon Composites During Processing: Intelligent Processing of Materials; Eddy Current Sensing of Carbon-Carbon Composites During Processing; Development of Electromagnetic Probes for Intelligent Processing of Dielectric Materials; Transient Elastic Waves in Laminates; X-Ray Radioscopy Standards; Advancement of Documentary Standards for Nondestructive Evaluation; Eddy Current Standards and Methods; Ultrasonics and Acoustic Emission Standards and Methods; Nondestructive Evaluation Using Magnetic Particles Magnetic Particles.

100,996

Not available NTIS PB92-117027 National Bureau of Standards (NEL), Gaithersburg, MD. Automated Production Technology Div.

# Computer Aided Manufacturing (CAM)

Mare Island Flexible Manufacturing Workstation. Final rept.

K. Lee, and C. Lee. 1988, 10p

Sponsored by Naval Research Lab., Washington, DC. Navy Manufacturing Technology Program.

Pub. in Proceedings of International Conference on Computer Integrated Manufacturing, Troy, NY., May 23-25, 1988, p9-18.

Keywords: \*Computer aided manufacturing, \*Workstations, Automation, Robotics, Robots, Quality control, Reprints, NIST, Flexible manufacturing.

The Mare Island Flexible Manufacturing Workstation is being developed at the National Institute of Standards and Technology (NIST). Advanced features include hierarchical control architecture, combined machining and turning operations in one machine, adaptable workholding, flexible robot end-effector, robotic changing of tools, chuck jaws, and gripper fingers, robotic workpiece loading and unloading, and automated buffer storage of supplies. Quality control is achieved butier storage of supplies. Cutality control is achieved by using in-process gaging, tool setting, and tool con-dition monitoring. When completed, the Mare Island Flexible Manufacturing Workstation will be the first small-batch flexible manufacturing system in the U.S. capable of continuous unattended production of RISIC.parts.

100,997 PB92-123058 PC A03/MF A01 National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Factory Automation Systems Div. Multi-Enterprise Concurrent Engineering through International Standards.

G. P. Carver, and H. M. Bloom. Oct 91, 27p NISTIR-4708

See also PB91-193367.

Keywords: \*Computer aided manufacturing, \*Product development, \*Standards, Automation, Standardiza-tion, Data bases, Concurrent processing, \*Concurrent engineering, PDES(Product Data Exchange Using STEP), STEP(Standard for The Exchange of Product model data)

Concurrent engineering involves the integration of people, systems and information into a responsive, efficient system. Integration of computerized systems allows additional benefits: automatic knowledge capture during development and lifetime management of a product, and automatic exchange of that knowledge among different computer systems. Critical enablers are product data standards and enterprise integration frameworks. A pioneering assault on the complex technical challenges is associated with the emerging international Standard for the Exchange of Product Model Data (STEP). Surpassing in scope previous standards efforts, the goal is a complete, unambiguous, computer-readable definition of the physical and functional characteristics of a product throughout its life cycle. The use of STEP will lead to higher, integrated levels of automation based upon information standards and frameworks. Concurrent engineering, through information technology and standards, represents the power of a new industrial revolution.

## **Computer Software**

100,998 PB91-144378 PC A03/MF A01 National Inst. of Standards and Technology, Gaithers-

burg, MD.
NIST STEP Working Form Programmer's Reference. National PDES Testbed Report Series (Re-

vised). S. N. Clark. 29 Nov 90, 27p NISTIR-4353/REV See also PB90-250077.

Keywords: \*Standards, \*Computer \*Computer aided manufacturing, \*Computer aided design, "Computer aided manufacturing, Mathematical models, Computer software, Parsers, File structures, Translators, Computer programming, \*PDES(Product Data Exchange Specification), \*STEP(Standard for the Exchange of Product Model Data), National Institute of Standards and Toolpologic Standards and Technology.

The Product Data Exchange Specification (PDES) is an emerging standard for the exchange of product information among various manufacturing applications. The neutral exchange medium for PDES product models is the Standard for the Exchange of Product

Model Data (STEP) physical file format. The National PDES Testbed at the National Institute of Standards and Technology (NIST) has developed software to manipulate and translate STEP models. The software consists of an in-memory working form and an associated physical file parser, STEPparse. The internal operation of the STEPparse parser is described. The implementation of the data abstractions which make up the STEP Working Form is discussed, and specifica-tions are given for the Working Form access functions. The creation of STEP translators using STEPparse is discussed.

#### Job Environment

100,999

PB91-167403

PC A06/MF A01

National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Center for Fire Research. Users Guide for RAPID, Version 2.3.

Special pub. (Final).

R. D. Peacock, J. N. Breese, and C. L. Forney. Jan 91, 113p NIST/SP-798

Supersedes PB87-100996. Also available from Supt. of Docs. as SN003-003-03046-5.

Keywords: \*Fire tests, \*Data reduction, \*Computer applications, Data acquisition, Data processing, Data file, Input output processing, Utility routines, Digital command systems, User manuals(Computer programs), RAPID computer program.

The voluminous amount of data that can be collected by automatic data acquisition systems during large scale fire tests requires the use of a digital computer for the reduction of data. RAPID is a stand-alone program specifically designed to convert raw instrument voltages collected during such tests into a meaningful The reduced data can also be used alone or in combinations to obtain derived quantities. The program is written with the ability to accept data from a user defined data acquisition system and to check the correctness of data being analyzed. The data can be converted into meaningful scientific units and then presented in tabular or printer plot form, or stored for further processing. The guide provides detailed instructions for the use of the program.

101,000

PB91-184762 PC A03/MF A01 National Inst. of Standards and Technology (BFRL), Gaithersburg, MD.

Visibility of Exit Directional Indicators.

B. L. Collins, and P. J. Goodin. Mar 91, 44p NISTIR-4532 See also PB91-161984. Sponsored by National Electrical Mfrs. Association, Washington, DC.

Keywords: \*Emergency planning, \*Human factors en-

gineering, Display devices, Indicator lights, Safety, Vis-ibility, Human behavior, Luminance, Egress, Exit signs. A three-phase experiment assessed the effectiveness

of different configurations for exit signs and directional indicators. Two phases involved visibility assessments, while a third phase was a behavioral assessment. In the experiment, sign effectiveness was determined in terms of distance to detection, correct identification, and rated effectiveness, as well as speed through a corridor. The results indicated that a chevron in grey on white with a contrast of about 0.4 to 0.5 (to meet minimum specifications) was identified correctly at the greatest mean distance and received the highest mean ratings of effectiveness, as compared to other directional indicators. The combination of a 2.25in chevron with a 6-in EXIT sign was identified correctly at a mean distance of about 100 ft. Use of color, either red or green, increased the distance by about 15 to 20 ft. Visibility is best predicted by total chevron area, with chevrons with larger total areas seen at greater distances. Analysis of the movement data from the behavioral phase indicated that chevrons of 2.25-in provided adequate visibility at about 100 ft, but that speed of movement is not a sensitive indicator for sign visibili-ty. Finally, the data from all three phases indicate the importance of chevron size and configuration as well as sign color and contrast in determining visibility.

#### Joining

101.001

Not available NTIS PB91-134619 National Inst. of Standards and Technology (IMSE), Boulder, CO. Fracture and Deformation Div. Report on 1989 Actions by International Institute of Welding.

Final rept.

T. A. Siewert, and M. J. Houle. 1990, 3p Pub. in Materials Evaluation 48, p408, 411-412 Mar 90.

Keywords: \*Welding, \*Nondestructive tests, Standards, Reprints, \*Foreign technology, International Institute of Welding, International organizations.

The summary describes the activities at the 1989 meeting of the International Institute of Welding Commission V - Testing, Measurement, and Control of Welds. The summary makes U.S. industry aware of European research and standard development in this area, and solicits U.S. input for international documents.

101.002

PB91-149278 Not available NTIS National Inst. of Standards and Technology (IMSE), Boulder, CO. Fracture and Deformation Div. Dynamic Arc-Power Source Response in GMA

Welding. Final rept

T. A. Siewert, and G. Kohn. 1989, 4p

Pub. in Proceedings of American Welding Society Annual Meeting (68th) and International American Welding Society Brazing Conference (18th), Chicago, IL., March 22-27, 1987, p43-46 1989.

Keywords: \*Gas metal arc welding, \*Dynamic response, Weld metal, Welding current, Base metal, Electric current, Filler metal, Weldments, Welding, Re-

Previous studies of droplet transfer frequency in gas metal arc (GMA) welding have been reported primarily as a function of the welding current. The study investigates both current and voltage effects in the short circuiting mode and reports the additional effects of the power supply characteristics and other welding procedure parameters on the droplet transfer. A computer simulation of short-circuiting transfer has been developed. The effect of changes in the welding parameters in the model are compared to actual welds. The simulated weld data match the actual weld data to within

101.003

PB91-162339 Not available NTIS National Inst. of Standards and Technology (MSEL), Boulder, CO. Fracture and Deformation Div.

Analysis and Characterization of Commercial Welding Fluxes.

Final rept.

T. A. Sjewert, and G. L. Franke. 1990, 9p Sponsored by David Taylor Research Center, Bethesda. MD

Pub. in Welding Research Supplement, p247s-255s Jul 90

Keywords: \*Welding, \*Composition(Property), \*Spectroscopic analysis, X ray fluorescence, X ray diffraction, Fluxes, Welding rods, Welding electrodes, Chemical properties, Quality control, Reprints.

Various quantitative and qualitative flux analysis techniques were evaluated using a series of highly basic submerged arc welding fluxes. The test matrix included some replicate testing so the precision of the primary measurement techniques could be compared. The results indicate that optical emission spectroscopy can match the precision of x-ray fluorescence, while providing data on many more elements, some of which could be important monitors of the quality of the flux. X-ray diffraction and particle size analysis provide additional information that complement the compositional data provided by the first two techniques. The techniques were able to identify compositional variations that explained the difference in the color of two flux samples and revealed a composition change with particle size for one flux sample. For applications where a tighter control of flux composition is warranted, these techniques can provide quality control infor-mation beyond that provided by typical quality control

## Joining

101,004 PB91-174250 Not available NTIS National Inst. of Standards and Technology (MSEL), Boulder, CO. Fracture and Deformation Div. Sensing of GMAW Droplet Transfer Modes Using an ER 100S-1 Electrode.

Final rept. G. Adam, and T. A. Siewert. 1990, 6p Pub. in Welding Research Supplement, p103-s-108-s

Keywords: \*Gas metal ore welding, \*Control systems design, \*Computer applications, Welding current, Welding electrodes, Weld metal, Microcomputers, Computer aided manufacturing, Weldments, Statistical analysis, Sensors, Reprints.

The authors evaluated the capability of a 16-MHz microcomputer with a fast analog-to-digital conversion board to capture welding data and to develop throughthe-arc sensing and control parameters for the gas metal arc welding process. After software was customized for the application, current and voltage data at sampling rates up to 50 kHz could be recorded for relatively long times, limited only by available disk space. The analysis software enabled them to extract numerical data and manipulate it using statistical analysis. Fourier transforms, amplitude frequency histograms, peak-searching algorithms and smoothing procedures. To determine the capabilities of the system, it was applied to the study of welding with an ER100S-1 electrode. The current and voltage were recorded for 197 welds which formed a matrix of welding conditions encompassing short-circuiting, globular and spray transfer modes, as well as the transition regions between these modes.

#### Manufacturing, Planning, Processing & Control

PB91-162230 Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Factory Automation Systems Div.

Research Tackles Automation Issues. Final rept. C. R. McLean. 1986, 5p Pub. in Design News 7, p94-98 Jul 86.

Keywords: \*Automation, \*Manufacturing, \*Technology utilization, Industrial plants, Research projects, Computer aided manufacturing, Fabrication, Assembly lines, Production management, Industries, Production engineering, Reprints, \*Automated Manufacturing Research Facility.

Major technical obstacles have inhibited the spread of automation within key sectors of American industry. Factory automation researchers at the National Bureau of Standards in Gaithersburg, Md. are working on overcoming some of those obstacles. A small batch manufacturing system testbed, the Automated Manu-facturing Research Facility (AMRF), currently under construction at the National Bureau of Standards (NBS), is designed to support research in factory automation standards. The article briefly describes the technical obstacles inhibiting factory automation, the goals of the project, key participants, system concepts, and the architecture of the AMRF testbed.

PB91-240812 PC A04/MF A01 National Inst. of Standards and Technology (MEL), Gaithersburg, MD. New Concepts of Precision Dimensional Measure-

ment for Modern Manufacturing. D. A. Swyt. Aug 91, 59p NISTIR-4644

Keywords: \*Manufacturing, \*Dimensional measurement, Error analysis, Accuracy, Precision, Machine tools, Length, Distance measuring equipment.

A new scheme for the analysis of the origin and propogation of errors in length-based dimensions is presented, one which is applicable to the characterization of measuring machines, machine tools, and the dimensioned parts which they characterize or form. The scheme involves a matrix of four dimensional-type-specific errors (associated with the length-based quantities of displacement, position, distance and extension) and three measurement-axiom-specific errors (associated with rules governing the zero, the unit and the scale of measurement). Application of the scheme is illustrated by a propogation of error analysis of the use of a laser-interferometer-based coordinate meas-uring machine for the determination of the length of a simple part. Also indicated is how an identical analysis applies to the characterization of the performance of machine tools which shape such parts.

#### **Optics & Lasers**

PB91-162107 Not available NTIS National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Ceramics Div.

Analytic Solution for the Three-Layer Multiple Beam Interferometer. Final rept.

R. G. Horn, and D. T. Smith. 1991, 7p Contract ONR-N0014-8-F-0034
Sponsored by Office of Naval Research, Arlington, VA.

Pub. in Applied Optics 30, n1 p59-65, 1 Jan 91.

Keywords: \*Interferometers, Diffraction patterns, Coatings(Materials), Silver, Silica, Sapphire, Mica, Thin films, Measurement, Analytical solution, Metal films,

A simple analytic solution for the condition of constructive interference for light transmitted through an interferometer incorporating three ideally transparent layers of arbitrary thickness and refractive index is pre-sented. Also considered are the effect of adding two metallic coatings to the outer surfaces of the interferometer and empirical expressions for the associated phase changes for silver coatings on silica, sapphire, and mica substrates. A particular application to fringes of equal chromatic order can be utilized to obtain precise measurements of the thickness of extremely thin films sandwiched between two substrates.

## **Quality Control & Reliability**

101,008 PB91-143339 PC A05/MF A01 National Inst. of Standards and Technology (MSEL), Gaithersburg, MD.
Materials Reliability. Technical Activities, 1990.
(NAS-NRC Assessment Panel, January 31-February 1, 1991). H. I. McHenry. Dec 90, 82p NISTIR-90/4395

Keywords: \*Research projects, \*Reliability, Aircraft construction materials, Ultrasonic tests, Nondestructive tests, Polymer-matrix composites, Greens function, US NBS, Cryogenics, Aluminum alloys, Thermomechanical treatment, Lithium alloys, Packaging, Soldered joints, Stress analysis, Steels, Charpy impact test, Standards, Arc welding, Super conductors.

Selected Highlights of the Materials Reliability Division are as follows: Composites NDE: A high resolution ultrasonic system has been developed for inspecting thick polymer-matrix composites; NDE Instruments: Field trials were conducted on two prototype ultrasonic NDE instruments. A formability sensor system was de-livered to the Ford Motor Company for evaluation at their Dearborn stamping plant. An ultrasonic system for roll-by inspection of railroad wheels is being evalu-ated at the American Association of Railroads test track in Pueblo, Colorado, Elastic Waves in Compos-ites: A powerful technique using a time-dependent Green's function method has been developed for studying propagation of elastic waves and their scatstudying propagation of elastic waves and fileli scattering from discontinuities in anisotropic solids; Electronic Packaging: Computer programs have been developed to convert coordinate points on solder joint surfaces obtained by x-ray laminography and optical inspection into finite element meshes for stress analysis. The programme and processing the programme of the programme in the programme sis; Thermomechanical Processing: The continuous cooling transformation (CCT) characteristics and the high-temperature, high strain-rate flow properties were measured for microalloyed SAE 1141 forging steel; Charpy Standards: Over 1000 industrial customers were supplied with Charpy V-notch reference specimens and calibration services for certification of Charpy impact test machines to ASTM Standard E23;

Cryogenic Testing: A 5 MN (1 million pound-force) servohydraulic testing machine was refurbished and equipped with a cryostat and dewar capable of testing specimens 2 m long and 50 cm in diameter in liquid helium; Aluminum-Lithium Alloys: A cooperative pro-gram with NASA indicated that aluminum-lithium alloys have sufficient oxygen compatibility for use in cryogennave sufficient oxygen compatibility for use in cryogen-ic tankage for the Advanced Launch System; Automat-ed Welding: An intelligent welding program was initiat-ed for the U.S. Navy in conjunction with Babcock and Wilcox and INEL; and Superconductors: Using an ionic-crystal model and ultra sound-velocity measure-ments, some physical properties of the Y1Ba2Cu3Ox superconductor were studied as a function of oxygen content (x — 8-7) content (x = 6-7).

101,009 PB91-147132 PB91-147132 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Radiometric Physics Div. Fundamentals and Applications of Infrared Thermography for Nondestructive Testing. Final rept.

Final rept.

Pub. in International Advances in Nondestructive Testing, v13 p39-81 1987.

Keywords: \*Nondestructive tests, \*Infrared thermography, \*Thermography, Temperature measurement, Thermal radiation, Imaging techniques, Reprints.

The recent availability of highly sophisticated thermal imaging systems, in particular, digitized scanners with storage and computational capabilities, has engendered a rash of new NDT applications for infrared thermography which pervades industry. The paper treats two areas: fundamental physical concepts of infrared thermography, which provides the rationale for experimentation and pallipations of thermography. mentation, and applications of thermography to NDT. Topics included in the former area are thermal radiation; thermal imaging systems, their operation, performance characteristics, and external influences; targets; and radiation thermometry. The latter area is a critical review of applications literature, with emphasis on the 'new thermography' and with examples selected to illustrate new trends and techniques.

101,010 PB91-147900 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Ionizing Radiation Div. Real-Time Radiology Standards: Results of a

Workshop.

Final rept. R. C. Placious, and T. A. Siewert. 1987, 2p Pub. in Materials Evaluation 45, p1270-1271 Nov 87.

Keywords: \*Radiology, \*Radiography, \*Standards, Real time, US NBS, Meetings, Reprints.

A two day workshop was held recently to review National Bureau of Standards (NBS) activities in real-time radiology, to obtain the opinion of experts on stand-ards needs in the rapidly developing technology, and to guide NBS in identifying, in order of priority, those activities that would most benefit the industry.

PB91-148163 Not available NTIS National Bureau of Standards, Gaithersburg, MD. Program Office. Industry and Government Strategies for Product

Quality. Final rept.

G. Tassey. 1989, 15p Pub. in International Jnl. of Technology Management 4, n2 p189-203 1989.

Keywords: \*Quality, \*Product development, Government policies, Industries, Technology innovation, Competition, Manufacturing, Reliability, Marketing, Re-

Quality has become an increasingly important part of competitiveness strategies in the United States and other nations. Yet, the concept of quality and the approaches to implementing strategies to improve quality are not well developed. In particular, the term quality connotes to many a highly subjective image in which qualitative reactions by customers is the primary measuring stock. Views on the barriers to achieving higher levels of quality suffer from a signular focus on higher levels of quality suffer from a singular focus on technical or organization factors. Quality in manufac-tured products is a combination of performance levels, performance stability, reliability, and longevity. Ad-

## **Quality Control & Reliability**

vancing any or all of these elements of quality requires a range of technological, organizational, and marketing changes. Specific technical solutions cannot be effectively conceived and implemented in isolation from the broader system of production and servicing of targeted markets. This implies a trend toward integration of research and development, production, and marketing. Moreover, an increasing fraction of technical solutions will have to come from outside the corporate entity as will information on the broader technological and market trends.

101.012

PB91-149088 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD.

NBS Quality Assurance Support: Current and Planned Services.

Final rept.

C. W. Reimann. 1986, 9p Pub. in Proceedings of American Society for Quality Control, Annual Quality Congress Transactions (40th), Anaheim, CA., May 19-21, 1986, p53-61.

Keywords: \*Quality assurance, \*US NBS, Measurement, Calibration, Uses, Reprints, \*National Bureau of Standards, Reference materials, US NIST.

The National Bureau of Standards (NBS) is the central reference laboratory for the U.S. that provides measurement services - calibrations, standard reference materials, and standard reference data - for process and quality control applications, adaptable to a wide range of technologies and quality assurance management systems. Measurement provides a quantitative foundation for quality assurance. Chemical and physical tests are used increasingly throughout the cycle of production and plant operations, and measurement now represents a significant manufacturing cost element. While measurement science has made enormous gains, the state of measurement practice lags in many areas. Despite the growing need for reliable measurement, there are a number of barriers to wider use of standards and related quality assurance services. Cooperative projects and broader community input to NBS priorities offer avenues to improve use of NBS quality assurance services and to stimulate the development of needed services. The paper summarizes growing application areas, measurement trends, NBS' current services and plans, and outlines mechanisms for effective interaction with NBS.

## 101.013

PB91-149930 Not available NTIS National Bureau of Standards (NML), Gaithersburg,

Measurement Quality Assurance.

Final rept. C. W. Reimann. 1987, 10p

See also PB89-147508.

Pub. in Proceedings of American Society for Quality Control Annual Quality Congress Transactions (41st), Minneapolis, MN., May 4-6, 1987, p389-398.

Keywords: \*Quality assurance, \*US NBS, Measurement, Calibration, Uses, Reprints, \*National Bureau of Standards, Standards laboratories, US NIST, Traceability.

Measurements in the U.S. economy now cost more than \$200B annually. The principal uses of measurements are as appraisal tools in quality assurance applications affecting products, processes, environmental quality, and health care. High technology areas such as advanced materials, aerospace and defense systems, opto-electronics, and biotechnology incur measurement costs three to five times higher than such costs in traditional technologies. In addition, high technology areas demand greater accuracy, in many cases challenging state-of-the-art capabilities. The paper summarizes the rationale for measurement quality, key elements contained in such a system, linkages be-tween standards laboratories and plant operations, and the role of the National Bureau of Standards (NBS). The paper will include an update of services available from NBS to support corporate quality assur-

## 101.014

PB91-159103 Not available NTIS National Inst. of Standards and Technology, Gaithers-burg, MD. Standard Reference Materials Program.

Reference Materials: Their Role in Measurement Accuracy.

Final rept. W. P. Reed, and S. D. Rasberry. 1990, 9p Pub. in Impact of Science on Society, n157 p71-79

Keywords: Materials tests, Measurement, Accuracy, Reprints, \*Reference materials, US NIST.

Measurement compatibility and the establishment of production standards are very important aspects of manufacturing, material processing, and environmental monitoring. Organizations such as the US National Institute of Standards and Technology play a key role in providing the wide variety of reference materials required.

101,015 PB91-162354 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Precision Engineering Div. Stylus Profiling at High Resolution and Low Force. Final rept. J. F. Song, and T. V. Vorburger. 1991, 9p

Keywords: Gratings(Spectra), Calibration, Surface roughness, High resolution, Diamonds, Pens, Reprints, \*Atomic force microscopy, \*Profilometry, Styluses.

Pub. in Applied Optics 30, n1 p42-50, 1 Jan 91.

The paper describes experimental work to improve the lateral resolution of stylus instruments. The efforts involve (1) use of a fine stylus, (2) low stylus load, (3) high magnification in the lateral direction, and (4) specimens with fine surface structure by which the lateral resolution of stylus instruments could be detected. By using styli with tip widths between 0.05 and 0.15-micrometer a stylus load of 0.6-1.2  $\times$  10 to the -6 power N (0.06-0.12-mgf), and a piezostage for lateral dis-placement, the authors detected 0.05-0.15 micrometer lateral resolution on the surfaces of different kinds of specimens. To get a high lateral resolution, the most important consideration is a fine stylus with small tip

101,016 PB91-167221 PC A03/MF A01 National Bureau of Standards (NEL), Gaithersburg, MD. Machine Intelligence Group.

Review of Current Geometric Tolerancing Theo-

rles and Inspection Data Analysis Algorithms S. C. Feng, and T. H. Hopp. Feb 91, 24p NISTIR-4509

Sponsored by Naval Research Lab., Washington, DC. Navy Manufacturing Technology Program.

Keywords: \*Dimensional measurement. \*Tolerances(Mechanics), State of the art, Computer aided design, Computer aided manufacturing, Inspection, Algorithms, Reviews, \*Coordinate measuring ma-

The report provides an overview of the state of the art in mechanical dimensioning and tolerancing theories and CMM inspection data analysis technology. It is expected that the information included in this review will benefit CMM software developers, CMM users, and researchers of new CMM technology. The document is the result of a survey of published geometric dimensioning and tolerancing theories and post-inspection data analysis algorithms. Both traditional and modern theories have been reviewed. Principles on which current national standards and international standards based have been stated. These geometric dimensioning and tolerancing principles are commonly used in mechanical design and part inspection. Post-inspec-tion data analysis algorithms, used for extracting features and evaluating tolerances, have also been reviewed. The effects of using different fitting criteria are discussed. From the theory and algorithm review, the authors recommend directions for future development in these areas. The bibliography covers activities and accomplishments of the research in advancing inspection technology.

PB91-187765 PC A03/MF A01 National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Robot Systems Div. AMRF Composites Fabrication Workstation: A

Test Methodology to Measure the Quality of Thermoplastic Composite Parts.
J. A. Falco. Apr 91, 23p NISTIR-4552

Keywords: \*Composite fabrication, \*Nondestructive tests, Composite materials, Workstations, Robotics,

Manipulators, Consolidation, Reinforced plastics, Quality control, Inspection, Methodology, Automated Manufacturing Research Facility, Thermoplastic composites.

The Robot Systems Division of the National Institute of Standards and Technology (NIST) requires a test methodology to measure the quality of the composite parts produced by an advanced manufacturing work-station being assembled in the Automated Manufac-turing Research Facility (AMRF). The workstation will be used to study methods of fabricating complex shaped, continuous carbon fiber reinforced, thermoplastic composite parts using pre-impregnated tow. The paper discusses the mechanisms of thermoplastic consolidation and the various defects associated with poor consolidation. Several testing techniques are discussed concerning their ability to locate, identify and/ or quantify these defects. The discussion is followed by a trade off analysis of all considered testing techniques in an attempt to determine the most effective test methodology to measure the quality of thermoplastic composite parts.

101,018

PB91-190058 Not available NTIS National Inst. of Standards and Technology (MSEL), Boulder, CO. Fracture and Deformation Div. Image Quality Indicator Design for Radioscopy and Tomography.

Final rept. T. A. Siewert, D. W. Fitting, D. A. Shepherd, M. W. Austin, and C. N. McCowan. 1990, 8p Pub. in Review of Progress in Quantitative Nondestructive Evaluation, v9 p383-390 1990.

Keywords: \*Tomography, Monte Carlo method, X-ray imagery, Radiation transport, Image analysis, Resolution, Reprints, \*Image quality indicators, \*Radioscopy.

A new image quality indicator design is proposed for real-time radioscopy systems. The design has spherical symmetry, so it provides the same image quality information independent of rotation. The resolution of several prototype indicators was measured by image analysis of a fine-grained radiograph. The resulting image intensity profile was compared to a radiation transport model.

101,019

Not available NTIS PB91-194993 National Inst. of Standards and Technology (NEL), Gaithersburg, MD.

Process Quality Enhancement for Machine Tools: Measurements and Standards.

Final rept.

J. W. Lyons. 1989, 11p

Pub. in Proceedings of U.S.-China Science, Technology, and Economic Development Program - Technical Transformation of Traditional Industries, May 1988, p70-80 1989.

Keywords: \*Quality assurance, \*Process control, \*Process computers, Machine tools, Measurement, Standards, Mathematical models, Error correcting devices, Error detection codes, Reprints.

A careful study of three-dimensional coordinate measuring machines (CMM) has been made to ascertain the errors inherent in the machines and to learn how to provide measurement services for such devices. The errors in such machines are largely repeatable, systematic errors; the random errors are generally much smaller. Improved performance can be achieved with these machines by measuring the systematic errors and then removing them by adding corrections to the control computer. Next, the similar but more difficult problem of error determination and correction for cutting machines was considered. Besides the quasistatic errors found in the CMMs there are additional dynamic errors, principal among which are from ther-mal gradients arising in spindle bearings and other points of friction. Ways were devised to compute these errors from real-time sensory information combined with stored data on machine behavior and, also in real time, to add correction information to the control sig-nals. Ultimately, quality assurance for dimensions of parts will be attained in the factory of the future by an extension of the above approach rather than by postproduction gaging. The computer is making it possible to understand the behavior of the process machines and to use mathematical models of this behavior in the process control computers so that the machines are self-correcting and must perform within the specified control limits.

# MANUFACTURING TECHNOLOGY **Quality Control & Reliability**

PB91-203463 Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Precision Engineering Div. Capacitance versus Stylus Measurements of Sur-

face Roughness. Final rept.

A. G. Lieberman, T. V. Vorburger, C. H. W. Giauque, D. G. Risko, R. Resnick, and J. Rose. 1988, 16p Pub. in Surface Topography 1, p315-330 1988.

Keywords: \*Surface roughness, Mathematical models, Capacitance, Profiles, Probes, Metals, Pens, Reprints, Styluses.

Roughness measurements were performed upon a large variety of mechanical metal surfaces using capacitance roughness gauges and high-quality stylus in-struments. Profile measurements obtained from the stylus instruments served as the basis for modeling the response of the capacitance gauge to the surfaces. The probing element of the capacitance gauges consisted of a  $2.0 \times 16.8$  mm flexible platen, which, together with the rough metal surface, formed an electrical capacitor. Modeling the probe involved a detailed understanding of (1) how each element of the rough surface affects the sensed capacitance and (2) the way the flexible platen rests on top of the highest peaks of the surface and sags between these peaks. The model was realized as a FORTRAN computer program that uses a digitized stylus-generated profile as input data and computes the capacitive-roughness parameter R(c) as output. The model was validated by comparing the computed value of R(c) to that measured using the capacitance gauge for each of 41 different surfaces. The correlation of R(c) with more traditional definitions of roughness is also addressed for these same surfaces.

101 021 PB91-216721

(Order as PB91-216705, PC A07/MF A01) National Inst. of Standards and Technology, Gaithers-

burg, MD. Standard Reference Specimens in Quality Control

of Engineering Surfaces.
J. F. Song, and T. V. Vorburger. 1991, 19p
Included in Jnl. of Research of the National Institute of Standards and Technology, v96 n3 p271-289 May/Jun

Keywords: \*Surface roughness, \*Quality control, Calibration, Standard reference materials.

In the quality control of engineering surfaces, the authors aim to understand and maintain a good relationship between the manufacturing process and surface function. This is achieved by controlling the surface texture. In the paper, the characteristics, utilizations, and limitations of different classes of precision roughness calibration specimens are described. A measuring procedure of engineering surfaces, based on the calibration procedure of roughness specimens at NIST, is proposed. This procedure involves utilization of check specimens with waveform, wavelength, and other roughness parameters similar to functioning engineering surfaces. These check specimens would be certified under standardized reference measuring conditions, or by a reference instrument, and could be used for overall checking of the measuring procedure and for maintaining accuracy and agreement in engineering surface measurement.

101.022

PC A08/MF A02 PB92-112416 National Inst. of Standards and Technology (TS), Gaithersburg, MD. Weights and Measures Program. Uniforms Laws and Regulations as Adopted by the National Conference on Weights and Measures (76th), 1991. Handbook.

C. S. Brickenkamp, and J. A. Koenig. Oct 91, 173p NIST/HB-130-1992 ED Also available from Supt. of Docs. as SN003-003-03105-4. Supersedes PB91-107102.

Keywords: \*Weight measurement, \*Law(Jurisprudence), \*Regulations, \*Handbooks, Automotive fuels, Consumer affairs, Packaging, Standmeasurement,
\*Handbooks, ardization, Commodities, Prices, Labels, Food, Sales, \*Weights and measures, Weightmaster law, Open dating. Unit pricing.

The handbook, which is revised annually, compiles the uniform laws and regulations developed by the Committee on Laws and Regulations of the National Conference on Weights and Measures (NCWM). The compilation itself was approved by the NCWM in 1979, and the edition includes amendments adopted by the Conference at its annual meeting in 1991. The edition also contains an updated reprint of Section 2 from NCWM Publication 3, 'Policy, Interpretations, and Guidelines.' The NCWM recommends adoption and promulgation by the States of these uniform laws and regulations as updated in the handbook.

101,023

PB92-112424 PC A10/MF A03 National Inst. of Standards and Technology (TS), Gaithersburg, MD. Weights and Measures Program. Specifications, Tolerances, and Other Technical Requirements for Weighling and Measuring Devices as Adopted by the 76th National Conference on Weights and Measures, 1991. Handbook.

H. V. Oppermann. Oct 91, 214p NIST/HB-44-1992

Also available from Supt. of Docs. as SN003-003-03114-3. Supersedes PB91-107136.

Keywords: \*Measuring instruments, \*Weight indicators, \*Handbooks, Tolerances(Mechanics), Volume unit meters, Dimensional measurement, Specifications, Length, Odometers, Liquids, Vapors. 1251) Grain moisture, Taximeters.

Handbook 44 was first published in 1949, having been preceded by similar handbooks of various designations and in several forms beginning in 1918. The 1992 edition was developed by the Committee on Specifications and Tolerances of the National Conference on Weights and Measures with the assistance of the Office of Weights and Measures of the National Institute of Standards and Technology. It includes amendments adopted by the 76th annual meeting of the National Conference on Weights and Measures in 1991. Handbook 44 is published in its entirety each year following the annual meeting of the National Conference on Weights and Measures.

101,024

PB92-112465 PC A16/MF A03 National Inst. of Standards and Technology (TS), Gaithersburg, MD. Weights and Measures Program. Report of the National Conference on Weights and Measures (76th). Held in Philadelphia, PA. on July 14-19, 1991.

Special pub. (Final).

C. S. Brickenkamp, and A. H. Turner. Sep 91, 374p NIST/SP-816

Also available from Supt. of Docs. as SN003-003-03115-1. See also report for 1990, PB91-112763. Library of Congress catalog card no. 26-27766.

\*Weight measurement, \*Regulations, \*Meetings, Automotive fuels, Consumer affairs, Tolerances(Mechanics), Law(Jurisprudence), Railroad tracks, Food packaging, Measuring instruments, Standardization, Specifications, Commodities, Metrology, Training, Safety, \*Weights and measures, National Type Evaluation Program, NTEP program.

The theme of the 76th Annual Meeting of the National Conference on Weights and Measures (NCWM) was Weights and Measures for the Twenty-first Century. In the address to the delegates, Chairman David Smith of Nospection Service and NCWM joint program; the National Type Evaluation Program; and the needs for State metrology. Special meetings included those of the Metroligists, the Associate Membership Committee, the Retired Officials Committee the Scale Manufacturers' Association, the American Petroleum Insti-tute, the Industry Committee on Packaging and Labeling, the State regional weights and measures associations, and the National Association of State Departments of Agriculture Weights and Measures Division, and the National Council on State Metrication. Reports by the standing and annual committees of the Conference comprise the major portion of the publication, along with the addresses delivered by Conference officials and other authorities from government and indus-

#### Research Program Administration & Technology Transfer

PB91-149351 Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Center for Mfg. Engineering. Transferring NBS Technology to Small Manufacturers Through State and Local Centers.

Final rept.
D. A. Swyt. 1988, 7p
Pub. in Jnl. of Technology Transfer 13, n1 p7-13 1988.

Keywords: \*Technology transfer, \*Small businesses, Manufacturers, Government/industry relations, Robotics, Reprints, Automated Manufacturing Research Fa-

The paper provides a model of a technology-transfer system in which a federal laboratory -- the National Bureau of Standards's Automated Manufacturing Research Facility -- is linked to small manufacturers through state- and community-based technology centers, where the various institutions in the system are matched along dimensions of: level of government; stage in cycle of innovation; education of prototypical worker; and nature of capital-revenue base.

## Robotics/Robots

101.026

PB91-157214 PC A03/MF A01 National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Intelligent Controls Group.

TROI User's Guide.

B. Warsaw, and J. Michaloski. Jan 91, 46p NISTIR-

Keywords: \*Robots, \*Control systems, \*Man machine systems, Space stations, Man computer interface, User manuals(Computer programs), Real time systems, Interactive systems, \*TROI(TeleRobotic Operator Interface), Object-oriented programming.

The document provides an introduction to the TeleRobotic Operator Interface (TROI) system and a user guide to TROI programming and operation. TROI provides a flexible, extensible, object-oriented interface to the NASREM robot control system (RCS). It consists of two major portions, the X-window system Graphical User Interface (GUI), and the RCS's data-server interface modules. TROI provides a highly dynamic environment for interacting with the RCS. The user is able to view and modify state variables of a running control system, and to edit, save, and load graphical interface configurations while connected to a running control system. In this way, the user can interactively perform diagnostics, switch diagnostic contexts by creating and destroying interactive objects, and reconfigure data flow networks, allowing control of RCS operations without the costs of switching operating modes. TROI merges a user-initiated window system event model and an independent data driven event model into a single event stream.

101.027

PB91-158568 PB91-158568 Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Robot Systems Div. Self-Adjustment of a Robot Joint Controller.

Final rept.

N. Dagalakis, and D. R. Myers. 1986, 8p ber 1986, p530-537.

Keywords: \*Robots, \*Joints(Anatomy), \*Self adaptive control systems, Man machine systems, Optimization,

A self-adjustment technique based on performance A self-adjustment technique based on periorinance scheduling is applied to a robot joint controller. The technique allows a user to specify the desired time response of a joint to a step input. Using an optimization search routine the robot controller modifies its gain settings until its joint response matches the reference response. The adjustment technique has been tested on the wrist rotation joint of an industrial robot using a joint controller excitation and examination procedure

Robotics/Robots

previously developed at the National Bureau of Standards. The results indicate that the technique does permit the robot controller to modify joint response to match a user-specified desired performance.

101,028 PB91-158576 Not available NTIS National Bureau of Standards (NEL), Gaithersburg,

MD. Robot Systems Div.

Application of the Joint Excitation Gear Adjustment Technique to Low Frequencies and Heavy Robot Joints.

Final rept. N. G. Dagalakis, and D. R. Myers. 1987, 11p.

Contract N00014-83-K-0236 Sponsored by Office of Naval Research, Arlington, VA. Pub. in Proceedings of SME Conference on Robots, Chicago, IL., April 27-30-, 1987, p17-43-17-54.

Keywords: \*Robots, \*Gears, Performance evaluation, Adjusting, Accelerometers, Low frequencies, Reprints.

Previous work has demonstrated the use of the robot joint excitation technique and coherence analysis to adjust robot joint gears of light links for maximum precision. Band limited random joint motions are induced and the response of the link is monitored by one or more accelerometers. The gears are adjusted to minimize the effect of nonlinearities caused by backlash or tight meshing. The application of the technique to low frequencies and to heavy robot joints is examined. Experimental results are given from several robot adjust-ment tests as one recommendation for the easiest way to use this technique.

101,029 PB91-159194 Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Automated Production Technology Div.

Design and Implementation of a Five-Axis Robotic

Micromanipulator for Inserting Parts into Precision Collets. Final rept.

A. H. Slocum, L. Greenspan, and J. P. Peris. 1988,

9p Pub. in International Jnl. of Machine Tools and Manufacture 28, n2 p131-139 1988.

Keywords: \*Manipulators, \*Robotics, Servomechanisms, Hydraulic cylinders, Hydraulic motors, Degrees of freedom, Machine tools, Reprints.

The design, construction, and testing of a five-axis micromanipulator is described. It is designed to be attached to the end of a machine tool tending robot and to insert a part into a collet which is only 0.1 - 0.2 mm (.004 - .008 in) larger in diameter than the part; thus compensating for robot positioning errors. The micro-manipulator weighs 22N (5 lbs) and is 64mm (2.5 in) thick and 127mm (5 in) square with two linear axes with +/-3 mm (0.13 in) of travel, two angular axes with +/-4 angular degrees of motion, and one linear degree of freedom with +/-25 mm(1.0 in) of travel. Hydraulic actuators, with 6.9 MPa (1000 psi) fluid, provide 2700 N (600lbs) of force along the linear axes, and 68 N-m (600 in-lbs) of torque about angular axes. Repeatability of the device is .013mm (.0005 in).

101.030 PB91-167361 PC A03/MF A01 National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Robot Systems Div.

Robot Characterization Testing.

N. Dagalakis. Jan 91, 19p NISTIR-4510

Keywords: \*Robots, \*Characteristics, \*Performance evaluation, Tests, Manpower, Equipment, Capabilities, Standards, Parameter identification, Man machine sys-

The document describes the field of robot characterization which is broken into the areas of performance parameter identification, and environmental interaction. Each area is explored by considering the tests, equipment, and manpower required to characterize the capabilities and performance of robots.

PB91-174961 Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Robot Systems Div. Robot Sensor Language.

Final rept. S. Leake. 1987, 8p

Pub. in Proceedings of Goddard Conference on Space Applications of Artificial Intelligence (AI) and Robotics, Greenbelt, MD., May 13-14, 1987, p1-8.

Keywords: \*Robot sensors, \*Programming languages, Control systems, Syntax, Interactive systems, Algorithms, Debugging(Computers), Reprints, RSL(Robot Sensor Language).

Robot Sensor Language (RSL) is a data-driven, semiinterpreted, hierarchical, user extensible, robot task description language. It provides four levels of task decomposition, with structures and syntax specialized for each level. The user can add commands for new sensors appropriate to the task at hand. The language is highly interactive, easing debugging and algorithm development. It may also be used as an interface to a task planning system.

101 032 PB91-174979 Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Robot Systems Div.
Control of Flexible Robot Arm.

Final rept.

D. Lee, L. S. Haynes, B. L. Wang, and K. H. Tsai.

1987, 11p
Pub. in Proceedings of Conference on Modeling and Control of Robotic Manipulators and Manufacturing Processes, Boston, MA., December 13-18, 1987, p241-251

Keywords: \*Robot arms, \*Control systems, Computerized simulation, Sampling, Degrees of freedom, Damping, Reprints.

The work is a computer simulation of the control of the flexible robot arm. The dynamic equations for a singlelink flexible robot arm have been derived rigorously. The arm has two degrees of freedom in rotation and one in translation so that the workspace is three-dimensional. The payload is simulated by attaching additional mass to the arm at a specified location. The governing equations of the plant and the measurements are nonlinear. The process of control is divided into two stages: coarse control and fine control. Based on the pole-placement method, a linear observer is constructed for fine control. The numerical results of several cases are presented here. The effects of damping and sampling rate are also discussed.

101,033 PB91-194969 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Robot Systems Div. NASREM Robot Control System and Testbed. Final rept.

R. Lumia, J. Fiala, and A. Wavering. 1990, 7p Pub. in International Jnl. of Robotics and Automation 5, n1 p20-26 1990.

Keywords: \*Robots, \*Control systems, Hierarchies, Robotics, Manipulators, Remote sensing, Mathematical models, Algorithms, Test equipment, Reprints, \*NASREM, National Institute of Standards and Technology, National Aeronautics and Space Administra-

The National Aeronautics and Space Administration (NASA) National Institute of Standards and Technology (NIST) Standard Reference Model for Telerobot Control System Architecture (NASREM) provides the framework for a complete manipulator control system. It is composed of three hierarchies: task decompositris composed of three hierarchies: task deconliposi-tion, world modeling, and sensory processing. In the process of building NASREM, a great deal of effort has been spent in the definition of the interfaces between levels of the hierarchy so that the majority of robot control and sensory processing algorithms in the literature can be implemented. This allows the realization of the NASREM architecture to serve the dual purpose of robot controller and testbed for robot control algorithms. The paper describes the purpose and overall organization of NASREM. Then, two examples of NASREM task decomposition modules are discussed in terms of function as well as interface requirements.

PB91-203190 Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Robot Systems Div.

Application of the PIPE Image Processing Machine

to Scanning Microscopy. Final rept.

M. Herman, 1988, 5p Pub. in Proceedings of SPIE (Society of Photo-Optical Instrumentation Engineers) - Scanning Microscopy Technologies and Applications, Los Angeles, CA., January 13-15, 1988, v897 p169-173. Keywords: \*Robots, \*Computer vision, \*Image processing, Pipelining(Computers), Robotics, Microscopy, Scanners, Stereoscopy, Motion, Reprints.

PIPE is a pipelined image processing device that was designed for real-time robot vision applications. It accepts image from a video camera 60 times per second, and contains hardware for digitizing, displaying and performing operations on these images at video rates. Each stage of the pipeline contains arithmetic and logic units, convolvers, image buffers, and look-up tables. The purpose of the paper is to introduce PIPE and some of its applications to the scanning microscopy community. Three kinds of applications are described. The first is stereo analysis, whose purpose is to automatically extract range from two cameras mounted side by side. The second application is motion analysis and tracking. The application involves detecting motion, measuring its velocity, using it to obtain three-dimensional information, and tracking it through time. The final application is inspection of twodimensional patterns.

101,035

PB91-203208 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Robot Systems Div.

Video Compression for Remote Vehicle Driving. Final rept.

M. Herman, K. Chaconas, M. Nashman, and T. H. Hong. 1989, 8p

Pub. in Proceedings of SPIE (Society of Photo-Optical Instrumentation Engineers) - Mobile Robots III, Cam-bridge, MA., November 10-11, 1988, v1007 p136-143

Keywords: \*Robotics, \*Ground vehicles, \*Teleoperators, Image processing, Data compression, Real time, Remote control, Algorithms, Pipelining(Computers),

In order to effectively drive a remote ground vehicle using video images, the operator must be provided with a natural, real-time video sequence and the imagery must be accurate and detailed enough so that the operator can make mobility and survivability deci-sions. Unfortunately, high data rate communication channels are often not feasible for the task. To accomplish remote driving using a low data rate channel, video compression techniques must be incorporated. The paper discusses the remote vehicle driving problem and describes several video compression algorithms that have been implemented on PIPE, a realtime pipelined image processing machine. The paper then discusses how the algorithms are evaluated on real-world remote driving tests. Finally, advanced techniques for providing video compression are proposed.

101,036

PB91-217414 PC A03/MF A01 National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Robot Systems Div.

Generation of Smooth Trajectories without Plan-

J. C. Fiala. Jun 91, 19p NISTIR-4622

Keywords: \*Manipulators, \*Control systems, \*Trajectory control, Dynamical systems, Control theory, Robotics, Smoothing, Trajectory optimization, Robot dynamics, Simulation.

A technique for generating smooth trajectories of a system is presented. The approach is to find a dynamical equation with the desired transient behavior and use it as the basis of the control algorithm. It is shown that an appropriate dynamical equation can be obtained by varying the position and velocity gains of a proportional-derivative control loop over the duration of the movement. The dynamical equation can be used to generate trajectories online with minimal planning. The resulting manipulator control system responds to path errors in a more reasonable fashion than traditional approaches to trajectory control since explicit replanning is not required.

101,037

PB92-117019 Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Robot Systems Div.

#### Robotics/Robots

Performance Measures of a Robotic Micropositioner.

Final rept.

J. D. Lee, J. S. Albus, N. G. Dagalakis, and T. M. Tsai. 1988, 10p Pub. in Proceedings of International Symposium on

Robotics and Manufacturing: Research, Education, and Applications (2nd), Albuquerque, NM., November 16-18, 1988, p1047-1056.

Keywords: \*Robotics, \*Robot dynamics, \*Control systems, Computerized simulation, Robot arms, Manipulators, Algorithms, Positioning devices(Machinery),

The work describes a computer simulation of the dynamics and control of a robotic micropositioner. The robotic micropositioner is a parallel link manipulator which has six actuators, each controlled independently by a hydraulic system. The dynamic equations of the micropositioner are derived. The control algorithm for path tracing is formulated and tested. In the work, the performance of the micropositioner is investigated as a function of damping, speed, payload, and location of target.

## Tooling, Machinery, & Tools

101.038

Final rept.

PB91-146993 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Chemical Process Metrology Div. State-of-the-Art in Pressure Metrology.

V. E. Bean. 1990, 19p

Pub. in Proceedings of Symposium Semana de la Calidad y la Metrologia en El Politecnico, Mexico City, Mexico, November 26-30, 1990, p231-249 1990.

\*Pressure measurement, \*Metrology, \*Standards, State of the art, Manometers, Reviews, Reprints, Piston gages.

The state-of-the-art in pressure primary standards is reviewed. Among the areas that require continued research are: (1) The dependence of the effective area of a gas-operated piston gage on the gas species; (2) The dependence of the effective area of a gas-operated piston gage upon whether the gage is operated in the gage or absolute mode; (3) Methods for obtaining improved distortion coefficients for piston gages.

101.039

PB91-147751 Not available NTIS National Bureau of Standards (IMSE), Boulder, CO. Fracture and Deformation Div.

Progress in Uniform Field Eddy Current Methods.

Final rept. J. D. Moulder, N. Nakagawa, and P. J. Shull. 1987,

9p Contract W-7405-ENG-82

Sponsored by Air Force Wright Aeronautical Labs., Wright-Patterson AFB, OH. Materials Lab. Pub. in Review of Progress in Quantitative Nondestructive Evaluation, v7A p147-155 1987.

Keywords: \*Eddy current tests, \*Nondestructive tests, Electric current, Hysteresis, Magnetic fields, Eddy currents, Magnetic properties, Electrical properties, Field strength, Electromagnetic testing, Measuring instruments, Reprints.

The use of eddy current probes with a spatially uniform magnetic field distribution is especially advantageous for quantitative NDE, since the theoretical analysis of field-flaw interactions is much simpler for a uniform field. The authors reported here recent progress in the design and fabrication of high frequency uniform field eddy current probes. The goal has been to achieve higher frequency operation and greater bandwidth than previous designs so that smaller flaws may be studied over a greater range of skin depths. Measurements on artificial flaws designed to simulate crack 'bridging' phenomena are also described.

101,040

Not available NTIS PB91-158675 National Bureau of Standards (NEL), Gaithersburg, MD. Automated Production Technology Div.

Using Surface Roughness as a Wear Criterion in High-Speed Steel End-Milling. Final rept.

L. Evans. 1986, 6p
Pub. in Proceedings of North American Manufacturing Research Conference (14th), Minneapolis, MN., May 28-30, 1986, p177-182.

Keywords: \*Surface roughness, \*Machine tools, \*Wear, \*Steels, Machining, Surface properties, Finishes, Wear tests, Metal working, Reprints.

At the present time, there is no good quantitative wearout criterion that relates wear on the tool to the fitness of the tool for use in machining, and therefore no good one for tool wear testing. A criterion based on flank wear is commonly used but not universally accepted because it provides no indication of other kinds of wear occurring on the tool, and little information about the surface finish or dimensions of the machined part. It is important to choose a criterion related to the workpiece, since it is the quality of the part that matters. In the study, a wear-out criterion based on surface roughness is chosen and high-speed steel end-milling tests performed in order to judge the usefulness of the criterion. These tests do not monitor surface roughness inprocess; two indirect methods, feed force and cutting power, are studied as potential techniques to detect when a tool can no longer produce parts with a quality surface finish.

Not available NTIS PB91-159186 National Bureau of Standards (NEL), Gaithersburg, MD. Automated Production Technology Div. Kinematic Couplings for Precision Fixturing. Part

2. Experimental Determination of Repeatability and Stiffness.

Final rept.

A. H. Slocum, and A. Donmez. 1988, 8p Sponsored by Oak Ridge National Lab., TN. Pub. in Precision Engineering 10, n3 p115-122 Jul 88.

Keywords: \*Couplings, Fasteners, Stiffness, Precision, Test facilities, Ball bearings, Couplers, Fittings, Lubrication, Reproducibility, Reprints.

The paper describes results of tests performed to determine the repeatability of a large heavily preloaded kinematic coupling. The coupling was constructed from two 355.6 mm (14 in) diameter 101.6 mm (4 in) thick cast iron disks with hardened steel gothic archinserts and 28.6 mm (1.125 in) diameter balls. A special load frame was constructed for performing cyclic tests of kinematic coupling while applying a 5800 N (1300 lbh proload, Different types of balls and luthics). (1300 lbf) preload. Different types of balls and lubrication at the interface were tested. When using lubricated silicon nitride balls, axial and radial repeatability was on the order of 0.25 micrometers (+ or - 10 microinches). Stiffness was on the order of 180 kN/mm (10 (exp 6) lbf/in).

PB91-189225 Not available NTIS
National Inst. of Standards and Technology (NEL),
Gaithersburg, MD. Precision Engineering Div.
Statistical Process Control Tactics for Coordinate Measuring Machines.

Final rept.

T. Doiron. 1991, 12p

Pub. in Proceedings of Measurement Science Conference, Anaheim, CA., January 31-February 1, 1991,

Keywords: \*Dimensional measurement, \*Process control, Standards, Artifacts, Metrology, Accuracy, Reprints, \*Coordinate measuring machines, Gage blocks, Ball bars, Hole plates.

As coordinate measuring machines (CMMs) become the primary instruments for dimensional measurement in industry, the problem of process control for CMM accuracy is receiving increasing attention. While there is no obvious 'best' method for CMM statistical Process Control (SPC), there are a number of strategies based on the measurement of artifacts which are cur-rently in use. A number of these methods are presented, and their strengths and weaknesses are discussed with respect to accuracy, ease of use, reproducibility, flexibility, and response to common CMM problems.

101,043

PB91-202978 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Precision Engineering Div.

Computer Vision Based Station for Tool Setting and Tool Form Measurement.

Final rept. T. D. Doiron, 1989, 8p

Contract DE-Al05-85OR21584

Sponsored by Department of Energy, Oak Ridge, TN. Pub. in Precision Engineering 11, n4 p231-238 Oct 89.

Keywords: \*Computer vision, \*Tools, \*Metrology, Algorithms, Measuring instruments, Shape, gorithms, Measuring instruments, Snape, Position(Location), Accuracy, Workstations, Reprints.

The paper describes a computer vision based system which measures the shape of a turning tool edge and determines its position. The system consists of three subsystems: a computer vision system with a solid camera and microscope as the sensor, a metrology frame to provide scale and position information, and a set of algorithms to extract the needed information from the video output from the camera. The accuracy limitations of each subsystem are discussed and test data are compared with the accuracy predictions. The tool form measurements exhibited an accuracy which varied from 0.3 to 1.5 micrometers depending on the edge orientation. The tool setting accuracy was found to be near 2 micrometers. Suggestions for improvement are discussed.

101,044

PB92-123066 PC A03/MF A01 National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Factory Automation Systems Div. Use of Solid Modeling in the Design of M3 Components.

A. B. Feeney, and P. F. Brown. Sep 91, 35p NISTIR-4710

See also PB90-136938 and PB90-242207.

Keywords: Computer aided design, Vibration isolators, Dynamic control, Microelectronics, Metrology, Mass, \*Molecular measuring machines, Coordinate measuring machines, Solid modeling, Nanotechnology, M3

The paper documents the work done for the Molecular Measuring Machine (M3) Project by the Engineering Design Laboratory (EDL) at NIST. The M3 Project is developing and fabricating a device capable of making repeatable measurements of atomic scale features within a volume of 50mm x 100 micrometers. Extraordinary measures are being taken to isolate the device from mechanical vibrations, thermal loading and acoustic noise. The finest level of control over mechanical vibrations is achieved through an active vibra-tion isolation system. The EDL created solid models of the components and assemblies related to the active vibration isolation system in order to obtain the mass properties calculations required by the dynamic control system. The paper provides an overview of the M3 Project, describes the modeling work that was done within the EDL, and gives the mass property calculation results for the M3 parts and assemblies. Additionally, the paper discusses the advantages of using solid models as an integrated shape representation and a number of ways solid models are being used in product lifecycle applications.

#### **Tribology**

101.045

PB91-203943 Not available NTIS National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Ceramics Div. Numeric Database for Tribology: Format and Ap-

plication Issues. Final rept.

A. W. Ruff, J. Rumble, and S. Jahanmir. 1991, 17p Sponsored by Department of Energy, Washington, DC., National Science Foundation, Washington, DC., and Department of the Army, Washington, DC. Pub. in Computerization and Networking of Materials Databases: Second Volume, ASTM STP 1106, p180-106-1091

Keywords: \*Data bases, \*Tribology, Personal computers, Meetings, Friction, Wear, Mathematical models, Design criteria, Stress tests, Temperature dependence, Software engineering, Reprints, ACTIS data base.

Tribology

A computerized tribology information system designed for use with personal computers and including a numeric database is presently under development. The status of the system (named ACTIS) is summarized. Two important issues associated with the numeric database component were the data format and the organization of numeric data for user applications. Based on information developed at a National Institute of Standards and Technology (NIST) workshop on tribology information, a set of data fields has been identified for use in a database on friction and wear of materials, and on material properties. Evaluated data in these categories have been assembled and loaded into that format using commercial database manage-ment software. Over 360 records are presently contained in the database covering a broad range of materials of tribological significance. The data are orga-nized for direct application by the user in material selection, wear model calculations, tribological component design, and with other software codes such as stress and temperature calculations.

#### General

101,046 PB91-147942 Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Chemical Engineering Science Div. Review of Pulse Tube Refrigeration. Final rept.

R. Radebaugh. 1990, 15p

Sponsored by National Aeronautics and Space Administration, Moffett Field, CA. Ames Research Center. Pub. in Advances in Cryogenic Engineering 35, p1191-1205 1990.

Keywords: \*Refrigerators, \*Cryogenic cooling, Cryogenics, Stirling cycle, Coolers, Heat transfer, Refrigerating, Thermodynamic cycles, Efficiency, Mass flow, Pressure, Reprints, \*Pulse tube refrigerators.

The paper reviews the development of the three types of pulse tube refrigerators: basic, resonant, and orifice types. The principles of operation are given. It is shown that the pulse tube refrigerator is a variation of the Stir-ling-cycle refrigerator, where the moving displacer is substituted by a heat transfer mechanism or by an orifice to bring about the proper phase shifts between pressure and mass flow rate. A harmonic analysis with phasors is described which gives reasonable results for the refrigeration power yet is simple enough to make clear the processes which give rise to the refrigeration. The efficiency and refrigeration power are compared with those of other refrigeration cycles. A review is given of the research being done at various laboratories on both one and two-stage pulse tubes. A preliminary assessment of the role of pulse tube refrigerators is discussed.

101,047 PB91-147967 Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Chemical Engineering Science Div. Apparatus for the Measurement of Regenerator Performance in Pulse Tube Refrigerators. Final rept. W. Rawlins, and R. Radebaugh. 1990, 9p

Sponsored by National Aeronautics and Space Administration, Moffett Field, CA. Ames Research Center.
Pub. in Advances in Cryogenic Engineering 35, p1213-1221 1990.

Keywords: \*Refrigerators, \*Cryogenic cooling, \*Regenerators, \*Measuring instruments, \*Effectiveness, Coolers, Cryogenics, Mass flow, Heat loss, Heat exchangers, Cooling systems, Reprints, \*Pulse tube refrigerators.

The paper discusses the design and construction of an apparatus to measure the ineffectiveness of regenerators used for pulse tube refrigerators. Because of the fairly large mass flow rates which occur in pulse tube refrigerators, the regenerator ineffectiveness must be made quite small. The apparatus described here allows for the measurement of the regenerator's heat loss under actual operating conditions in a pulse tube refrigerator. A low temperature heat sink of liquid nitrogen is used since it approximates the temperatures normally achieved in a one-stage pulse tube.

101,048 PB91-187534

PC A05/MF A01

National Inst. of Standards and Technology (NEL), Boulder, CO. Chemical Engineering Science Div.

Analytical Model for the Refrigeration Power of the Orifice Pulse Tube Refrigerator. Technical note.

P. J. Storch, R. Radebaugh, and J. E. Zimmerman. Dec 90, 95p NIST/TN-1343

Also available from Supt. of Docs. Sponsored by National Aeronautics and Space Administration, Moffett Field, CA. Ames Research Center.

Keywords: \*Refrigeration, \*Mathematical models, \*Cryogenic cooling, Refrigerating, Refrigerating machinery, Coolers, Mass flow, Refrigerators, Cryogenics, Orifices, Pulses, \*Pulse tube refrigerators.

The pulse tube refrigerator is a cryocooler with potential for high reliability. The regenerative refrigerator op-erates with low average pressures, small compression ratios, and only one moving part. In research conducted at the National Institute of Standards and Technology, a pulse tube refrigerator with an orifice located at the closed, hot end of the system has been used to reach 60 K in one stage. A gross refrigeration power of 12 W has been measured at 80 K with a pulse tube volume of 30 cu m. The paper presents the develop-ment of an analytical model to predict the refrigeration power produced in an orifice pulse tube. Three versions of the model are presented: the first calculates quantities which are independent of dead volume; the second neglects dead volume; and the third describes a system with dead volume. Experimental results confirm predictions by the model that refrigeration power is proportional to the average pressure, the pulse frequency, the mass flow ratio, and the square of the dypressure ratio. Results are presented that are useful for approximate design of orifice pulse tube systems. The model assumes adiabatic conditions and an energy balance is performed in terms of net enthalpy flow. Phasor analysis was found to be very useful for analyzing the oscillations of pressure, temperature, and mass flow rate.

101.049 PB91-192997 PC A06/MF A01 National Inst. of Standards and Technology, Gaithersburg, MD. Office of Standards Services.

Conformity Assessment Workshop on Pressure

B. G. Simson. Apr 91, 103p NISTIR-4542 Sponsored by American Society of Mechanical Engineers, New York.

Keywords: \*Pressure vessels, \*Boilers, \*Meetings, Federal assistance programs, Government policies, European communities, Common market, Recommendations, Standards, International trade, Conformity as-

On January 31, 1991, The American Society of Mechanical Engineers (ASME) and the National Institute of Standards and Technology (NIST) cosponsored a workshop on pressure vessels at the Department of Commerce auditorium in Washington D.C. The purpose of the workshop, attended by one hundred and thirty two persons, was to explore how the U.S. Government can assist the pressure vessel industry in conformity assessment activities aimed at gaining acceptance of their products in such other markets as the European Community. The following recommenda-tions were reached by the private sector panelists: (1) U.S. Government promotion of national consensus standards; (2) enhancing NIST's standard information capability; (3) U.S. Government negotiation with the European Commission for establishing notified bodies for pressure vessels in the United States; and (4) U.S. Government establishment of a sectoral technical advisory organization.

101,050

PB91-194464 PC A05/MF A01 National Inst. of Standards and Technology (CSTL), Boulder, CO. Chemical Engineering Div. Heat Transfer and Pressure Drop in a Compact Pin-Fin Heat Exchanger with Pin Orientation at 18

deg to the Flow Direction.
D. A. Olson. Feb 91, 78p NISTIR-3965

Sponsored by National Aeronautics and Space Administration, Hampton, VA. Langley Research Center.

Keywords: \*Heat transfer, \*Pressure gradients, \*Friction factor, Turbulent flow, Reynolds number, Heat flux, Nusselt number, Heat exchangers, Temperature distribution, Experimental data, Mathematical models, \*Compact heat exchangers.

The authors have measured the heat transfer and pressure drop characteristics of a novel, compact heat exchanger in helium gas at 3.5 MPa and Reynolds numbers of 450 to 12,000. The 'pin-fin' specimen consisted of pins, 0.51 mm high and spaced 2.03 mm on centers, spanning a channel through which the helium flows; the angle of the row of pins to the flow direction was 18 degrees. The specimen was radiatively heated on the top side at heat fluxes up to 74 W/sq cm and insulated on the back side. Correlations were developed for the friction factor and Nusselt number. The Nusselt number compares favorably to those of past studies of staggered pin-fins, when the measured temperatures are extrapolated to the temperature of the wall-fluid interface.

101.051

PB91-203877 Not available NTIS National Bureau of Standards (NEL), Boulder, CO.

Chemical Engineering Science Div.

Optimization of a Pulse Tube Refrigerator for a Fixed Compressor Swept Volume.

Final rept.

R. Radebaugh, K. Chowdhury, and J. Zimmerman. 1988, 13p

Sponsored by National Aeronautics and Space Administration, Moffett Field, CA. Ames Research Center. Pub. in Proceedings of the International Cryocooler Conference (5th), Monterey, CA., August 18-19, 1988, p113-125.

Keywords: \*Cryogenic cooling, Refrigerators, Optimization, Cryogenic equipment, Refrigerating equipment, Cryogenics, Cooling, Ultralow temperatures, Refrigerating, Compressors, Cooling systems, Reprints, \*Pulse tube refrigerators

The paper discusses experiments which were done to determine the minimum temperature and the maxinum refrigeration power available with an orifice pulse tube refrigerator driven by a compressor with a fixed swept volume of 25 cu cm. The frequency of the compressor motion could be varied between 10 and 25 Hz. Only screen regenerators were studied but several mesh sizes and regenerator volumes were used. The screen materials tested were phosphor bronze, stainless steel, and nylon. Three different pulse tube volumes were investigated for most regenerators. The lowest temperatures achieved were about 67 K with the following conditions: pulse tube volume of 7.9 cu cm, regenerator gas volume of 9.2 cu cm, regenerator screen of 250 mesh stainless steel, frequency of 10-15 Hz, and average pressures of 1500-2000 kPa. These optimum volumes resulted in a pressure ratio of about

101.052

PB92-116482 Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Chemical Engineering Science Div. Measurement of Regenerator Performance in a Vuilleumier Refrigerator. Final rept.

P. E. Bradley, and R. Radebaugh. 1991, 10p Pub. in Proceedings of Interagency Meeting on Cryo-coolers (4th), Plymouth, MA., October 24, 1990, p195-204 1991

Keywords: \*Refrigerators, \*Performance evaluation. \*Regenerators, Cooling systems, Heat exchangers, Thermal efficiency, Mathematical models, Cryogenics, Low temperature tests, Refrigerating, Refrigerating machinery, Reprints, \*Vuilleumier refrigerator.

3-stage Vuilleumier refrigerator developed for Wright-Patterson Air Force Base has been used to measure the performance of third-stage regenerators. The refrigerator operates between 2.5 to 5.0 Hz and achieves temperatures of 10 to 20 K at the third-stage cold end. The purpose of the paper is to present a comparison of regenerator performance for two regenerator materials and to compare experimental results with a third order numerical model and a first order approximation for calculating the regenerator performance. Measurements of two regenerator materials are presented. Even though Brass has a volumetric heat capacity approximately 15 times lower than that of Pb+5%Sb, the regenerator loss with brass is only 60% higher than that of Pb+5%Sb because of the large heat capacity contribution of the helium gas in the regenerator void volume. These results are in fair agreement with a third order numerical model.

#### General

101,053 PB92-123041 PC A05/MF A01 National Inst. of Standards and Technology (MEL), Gaithersburg, MD.

Publications of the Manufacturing Engineering Laboratory Covering the Period January 1989-September 1991.

P. Nanzetta, C. F. Hutchins, and L. L. Wood. Nov 91, 95p NISTIR-4713

See also PB90-130568.

Keywords: \*Bibliographies, Dimensional measurement, Artificial intelligence, Production engineering, Automation, Metrology, Precision, Robotics, \*Manufacturing Engineering Laboratory.

The document provides a list of publications by staff of the Manufacturing Engineering Laboratory for the period of January 1989 through September 1991. Publications cover research done by the Laboratory in the areas of the precision dimensional measurement and precision engineering; robotics and intelligent machines; manufacturing data description, data administration, and information processing; and, sensors for manufacturing processes.

# MATERIALS SCIENCES

### Carbon & Graphite

101,054 PB91-158683 Not available NTIS National Inst. of Standards and Technology (MSEL),

Gaithersburg, MD. Ceramics Div.

Effects of Different CH4-H2 Gas Compositions on the Morphology and Growth of Diamond Grown by Hot Filament CVD.

Final rept.

E. N. Farabaugh, and A. Feldman. 1990, 6p Pub. in Materials Research Society Symposium Proceedings, v162 p127-132 1990.

Keywords: \*Diamonds, \*Thin films, Chemical vapor deposition, Crystal growth, Single crystals, Substrates, Methane, Hydrogen, Electron microscopy, Surface roughness, Process variables, X ray diffraction, Silicon, Mullite, Reprints.

Diamond films have been grown on single crystal Si and polycrystalline mullite substrates by hot filament chemical vapor deposition. Both substrates offer a good thermal expansion match with diamond. Gas mixture ratios of CH4:H2 ranged from 0.1-1.0%. The remaining deposition parameters were: substrate temperature, 750C; filament temperature, 1800C; gas pressure, 5000 Pa; gas flow rate, 52 sccm except for the 0.1% CH4:H2 ratio deposition in which the flow rate was 120 sccm. Film thicknesses were determined from cross sectional SEM micrographs. The average growth rates on the mullite increased nearly linearly with increasing CH4 gas fraction, ranging from 0.05 micrometers/hr to 0.21 micrometers/hr. Growth rates on the Si substrates were slightly lower for identical growth conditions. Surface SEM micrographs revealed that the rougness of the films decreased with increasing CH4 gas fraction during deposition. X-ray diffraction patterns showed that crystalline grain size in the films decreased with increasing CH4 gas fraction. No preferred crystallographic orientation was seen in the diffraction patterns.

PB92-116540 Not available NTIS National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Reactor Radiation Div. Neutron Measurements of Intramolecular Vibrational Modes in C60.

Final rept. R. L. Cappelletti, J. R. D. Copley, W. A. Kamitakahara, F. Li, J. S. Lannin, and D. Ramage.

1991, 4p Pub. in Physical Review Letters 66, n25 p3261-3264,

Keywords: \*Vibrational spectra, \*Carbon, Spectrum analysis, Neutron scattering, Measurement, Intramolecular structures, Reprints, \*Buckeyballs, \*Buckminsterfullerence.

Neutron-inelastic-scattering measurements have been made on a sample of highly purified solid C60. New features in the spectrum of intramolecular modes not obtainable by optical spectroscopy have been identified. Available theoretical calculations show trends in accord with the experimental results but disagree in important details, and improved calculations are desir-

## Ceramics, Refractories, & Glass

101,056 AD-A243 049/4 PC A08/MF A02 National Inst. of Standards and Technology (IMSE), Gaithersburg, MD. Ceramics Div. Strength and Microstructure of Ceramics. Final technical rept. 1 Oct 89-30 Sep 91. B. R. Lawn. Oct 91, 170p AFOSR-TR-91-0892, Grants AFOSR-ISSA-90-0003, AFOSR-ISSA-91-0002

Keywords: Aluminum oxides, Ceramic materials, Com-Keywords: Aluminum oxides, Ceramic materials, Composite materials, Cracks, Cycles, Degradation, Documents, Fatigue, Friction, Grain boundaries, Interfaces, Mechanical properties, \*Microstructure, Models, Predictions, Residual stress, Routing, Scanning electron microscopes, Strength(General), Test and evaluation, Theory, \*Ceramics, \*Strength(Mechanics), Grain size, Crystallization, \*Fracture(Mechanics), Toughness, Advanced composition, Craching Fracture (Mechanics), Cr vanced composites, Cracking(Fracturing), Scanning electron microscopy, Bridging, Tensile tests, Processing, Micromechanics.

Results of a program on the toughness properties of monophase and two phase ceramics that toughen by bridging are presented. Fracture mechanics models describing this behavior, in the particular context of strength, are developed. Results of strengths tests confirming the essential predictions of the theory are presented. Innovative processing routes suggested by the models are shown to lead to two phase compos-ites with impressive flaw insensitivity. A partial list of publications included in this report are: (1) The role of crystallization of an intergranular glassy phase in de-termining grain boundary residual stresses in debased aluminas; (2) In situ measurements of bridged crack interfaces in scanning electron microscopes; (3) Cyclic fatigue from frictional degradation at bridging grains in alumina; (4) Microstructure, toughness curves and me-chanical properties of alumina ceramics; (5) Fabrication of flaw tolerant aluminum titanate reinforced alumina; and (6) Influence of grain size and degree of crystallization of intergranular glassy phase on the mechanical behaviour of a debased alumina.

101,057 PB91-132233 PC A08/MF A01 National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Ceramics Div.
Institute for Materials Science and Engineering, Ceramics: Technical Activities 1990. S. M. Hsu. Nov 90, 170p NISTIR-4394 See also report for 1989, PB90-163981.

Keywords: \*Ceramics, Silicon nitrides, Phase dia-grams, Data retrieval, Standards, Superconductors, Thin films, Optical materials, Construction materials, Powder (Particles), Microstructure, Creep properties, Crack propagation, Surface energy, Glass, Data bases, Lubricants, Diamonds, Tribology, Characterization, Ceramic matrix composites, Fracture mechanics, Solid-solid interfaces.

Current programs of the Ceramics Division are reviewed. In 1990, technology transfer was accom-plished by the preparation and publication of 180 papers, the presentation of 150 talks and the submission of 6 invention disclosures. Leadership of national and international standards activities continued. The Structural Ceramics Database (SCD) Version 1.0 which contains evaluated thermomechanical data for industrial designers has been offered for public distribution by the Office of Standard Reference Data. Other database activities continued with the distribution of A Computerized Tribology Information System (ACTIS) and the completion of Volumes 7 and 8 of the NIST/American Ceramic Society Phase Diagrams for Ceramists. A new activity, an assessment of the New Diamond Technology in Japan was undertaken by division personnel in 1990. In the structural materials area, research on the chemistry of ceramic slurries and sus-pensions has led to identification of mechanisms for coating silicon nitride powders with discrete sintering aids. Significant advances in the ability to measure surface forces between dissimilar materials were achieved. Basic research on bridging effects in fracwere ture have been extended to microstructural design and studies of cyclic fatigue. Phase diagram determina-tions and studies of the role of processing environments on microstructural features of high temperature superconductors continued. The role of rare earth substitutions on YBaCO properties were evaluated and provided insight into the effect of atomic size of substitutional atoms.

PB91-147330 Not available NTIS National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Metallurgy Div. Dihedral Angles in Magnesia and Alumina: Distributions from Surface Thermal Grooves.

101,058

C. A. Handwerker, J. M. Dynys, R. M. Cannon, and R. L. Coble. 1990, 7p Pub, in Jnl. of the American Ceramic Society 73, n5 p1371-1377 May 90.

Keywords: \*Aluminum oxide, \*Magnesium oxides, \*Di-hedral angle, Grain boundaries, Polycrystalline, Sur-faces, Reprints.

Dihedral angles, psi, from surface thermal grooves were measured using a metal reference line technique for polycrystalline MgO, undoped Al2O3, and MgOdoped Al2O3. The values of psi, span the following ranges: 89 deg to 116 deg for MgO at 1520 K, 76 deg to 166 deg for undoped Al2O3 at 1870 K, and 90 deg to 139 deg for MgO-doped Al2O3 at 1870 K. The range of inclination angles of the grain boundary to the sur-face was a function of psi, with the maximum inclina-tion angle of about 13 deg, in quantitative agreement with theory.

101,059 PB91-147348 Not available NTIS National Inst. of Standards and Technology (MSEL),

Gaithersburg, MD. Metallurgy Div.

Metal Reference Line Technique for Obtaining Dihedral Angles from Surface Thermal Grooves.

R. L. Coble. 1990, 6p Pub. in Jnl. of the American Ceramic Society 73, n5 p1365-1370 May 90.

Keywords: \*Grain boundaries, \*Dihedral angle, Scanning electron microscopy, Aluminum oxide, Magnesi-um oxides, Grain growth, Surface energy, Reprints.

A metal reference line (MRL) technique is described for the measurement of surface-grain-boundary dihedral angles, psi, from thermal grooves at a sample surface using scanning electron microscopy (SEM). Metal lines deposited onto a thermally grooved surface using photolithography conform to the contours of the grainboundary groove and provide a high-contrast reference line for measuring psi, by SEM. Measurements of psi from optical interferometry and calculated from groove dimensions using surface diffusion models of thermal grooving are compared with the metal reference line measurements. ence line measurements from the same thermally grooved surface of MgO-doped Al2O3. Distributions of psi are found to shift to lower angles and approach the true psi value as the resolution of the technique increases, with the MRL technique having the highest resolution.

Not available NTIS PB91-147389 National Bureau of Standards (IMSE), Gaithersburg, MD. Ceramics Div.

Application of Analytical Electron Microscopy to Glass-Bonded Aluminas.

Final rept.

Pilia Tept.

B. J. Hockey. 1986, 4p
Proceedings of Annual Meeting Electron Microscopy
Society of America (44th), Albuquerque, NM., August
10-15, 1986, p436-439.

Keywords: \*Ceramics, \*Aluminum oxide, Electron microscopy, Electron diffraction, X ray analysis, Crystallization, Glass, Reprints.

The application of analytical electron microscopy to multi-phase ceramic materials is illustrated by studies

## **MATERIALS SCIENCES**

## Ceramics, Refractories, & Glass

on glass-bonded aluminas. Particular emphasis is placed on describing not only the morphology of the glassy intergranular phase, but its composition using energy dispersive X-ray analyses (EDX). Similarly, in conjunction with electron diffraction, is also used to determine the specific nature and distribution of intergranular crystalline phases that form as a result of devitrification during heat treatment of these alumi-

101,061 PB91-147553 Not available NTIS National Bureau of Standards (IMSE), Gaithersburg, MD. Ceramics Div.

Quantitative Determination of Amorphous Content in Ceramic Materials Using X-ray Powder Diffrac-

Final rept M. A. Kuchinski, C. R. Hubbard, L. A. Johnson, and V. A. Greenhut. 1988, 9p

Pub. in Proceedings of International Conference on Ceramic Powder Processing Science (1st), Orlando, FL., November 1-4, 1987, p321-329 1988.

Keywords: \*Ceramics, \*Amorphous materials, X ray diffraction, Cristobalite, Reprints, Powder diffraction.

quantitative technique which employs a modified method of additions approach to analyze for low amorphous content in crystalline matrices was developed and tested. Known amounts of amorphous material are added to the starting powder ('spiking'). The method uses the ratio of a measure of the intensity of the amorphous phase corrected for background to the background corrected intensity of a reference line from a crystalline phase. The amorphous spiking phase must be close in composition to the amorphous phase existing in the analyte. A critical step of the method is to correctly establish the background intensity. A completely crystalline material of similar scattering power was used to establish background intensity.

PB91-147983 Not available NTIS National Bureau of Standards (IMSE), Gaithersburg, MD. Ceramics Div.

Hermetically Sealed Inert Atmosphere Cell for X-ray Powder Diffraction. Final rept.

J. J. Ritter. 1988, 2p

Pub. in Powder Diffraction 3, n1 p30-31 Mar 88.

Keywords: \*X ray diffraction, \*Inert atmospheres, Hermetic seals, Barium oxides, Titanium boride, Reprints, Powder diffraction.

The construction and use of a captive inert atmosphere cell for the preservation of atmospherically sensitive samples during x-ray diffraction is described.

101.063 PB91-147991 Not available NTIS National Bureau of Standards (IMSE), Gaithersburg, MD. Ceramics Div.

Graphics Program for Binary and Ternary Ceramic Phase Diagrams. Final rept.

P. K. Schenck, and J. R. Dennis. 1987, 7p
Pub. in Proceedings of International Conference on
User Applications of Alloy Phase Diagrams, ASM Materials Week '86, Lake Buena Vista, FL., October 1986, p255-261 1987.

Keywords: \*Ceramics, \*Phase diagrams, \*Computer graphics, Computer applications, Data bases, Reprints.

The paper describes the computer graphics program developed for the National Bureau of Standards (NBS)
- American Ceramic Society (ACerS) Phase Diagrams for Ceramists Data Center for computer capture and reproduction of ceramic phase diagrams. The graphics program allows diagrams to be digitized, or entered by the keyboard, and provides a number of powerful editing features. The program produces publication quality diagrams for future volumes of 'Phase Diagrams for Ceramists'. The database of graphics files generated using the program will eventually be integrated with other databases under development in the Data Center, as described in a companion paper in the volume.

101 064 PB91-148221 Not available NTIS National Bureau of Standards (IMSE), Gaithersburg, MD. Ceramics Div.

Effects of Crystal Bonding on Brittle Fracture. Final rept.

G. S. White, E. R. Fuller, S. W. Freiman, and T. L. Baker. 1988, 7p

Pub. in Jnl. of Materials Research 3, n3 p491-497

Keywords: \*Ceramics, \*Semiconductors(Materials), \*Fracture mechanics, \*Brittle materials, Crack propagation, Indentation, Crystal structure, Environmental tests. Reprints.

Indentation techniques have been used both to obtain fracture energies as a function of board ionicity in various IV, III-V, and II-VI compounds and to determine the ability of environments to enhance crack growth in some of these materials. The fracture energies are compared to those obtained using a simplistic interplaner stress model and are found to agree within approximately 50%. Limitations of the indentation technique for evaluating n-values are discussed.

101,065 PB91-148767 Not available NTIS National Bureau of Standards (IMSE), Gaithersburg, MD. Ceramics Div.

Physical and Thermo-Mechanical Properties of Monoclinic Single Crystals.

Final rept. R. P. Ingel, P. A. Willging, B. A. Bender, and T. W.

Coyle. 1988, 11p Sponsored by Naval Research Lab., Washington, DC. Pub. in Advances in Ceramics 24A, p459-469 1988.

Keywords: \*Zirconium oxides, \*Ceramics, \*Single crystals, \*Monoclinic lattices, Electron microscopy, Temperature dependence, Mechanical hysteresis, Tetragonal lattices, Reprints, Thermomechanical properties.

Single crystals of unstabilized pure ZrO2 were successfully gorwn by the skull melting technique. TEM analysis revealed that the material was a monoclinic single crystal but heavily twinned with dislocations clearly visible. Physical property measurements (density, x-ray, etc.) were typical of monoclinic ZrO2. Strength and fracture toughness measurements as a function of temperature showed significant increases at 1200 C, just above the A(sub f) temperature of 1190 ACT The strength and toughness increased from 174 MPa and 2.4 MPam(Sup 1/2) at room temperature to 350 MPa and 5 MPam(Sup 1/2) at 1200 C. Testing at 1100 C showed large differences in behavior depending on whether the material was heated to the test temperature or cooled to the test temperature from the tetragonal phase field. These results indicate that there is a mechanical hysteresis which parallels the thermal expansion hysteresis. These effects are expected based on the stress-driven nature of the Monoclinic <-> Tetragonal transformation.

101.066 PB91-149096 · Not available NTIS National Bureau of Standards (IMSE), Gaithersburg, MD Ceramics Div

Low Temperature Chemical Process for Precursors to Boride and Carbide Ceramics Powders. Final rept.

J. J. Ritter, 1987, 21p

Pub. in Proceedings of Conference on Ceramic Powder Science and Technology, Boston, MA., August 6, 1986, 21p 1987.

Keywords: \*Ceramics, \*Precursors, \*Silicon carbides, \*Titanium borides, \*Boron carbides, \*Titanium borides, \*Boron carbides, Synthesis(Chemistry), Powder(Particules), Low tempersture, Reprints.

The controlled reductive dehalogenation of elemental halides has been studied as a low temperature approach to boride and carbide precursors. It was shown that TiCl4 and BCl3 react with metallic sodium at 130 C in a nonpolar solvent to give the precursor to TiB2. Similar type reactions with SiCl4 and CCl4 or with BCl3 and CCI4 have produced the precursors to SiC and B4C respectively. The chemistry is generally applica-ble to any combination of elemental halides which can be reduced by alkali metals or alkali metals alloys. The reactions in these systems are facilitated by highspeed, high-shear stirring and reaction temperatures of 110-130 C. Product NaCl is separated from the amorphous precursors by vacuum sublimation at 900 The TiB2 precursor undergoes initial crystallization at this temperature while the SiC precursor requires heating in excess of 1500 C to achieve crystallinity. The procedure has been successfully applied to the synthesis of precursors to the particulate composites SiC/TiC and SiC/TiN.

101.067

Not available NTIS PB91-149104 National Bureau of Standards (IMSE), Gaithersburg, MD. Ceramics Div.

Low Temperature Synthesis of Ceramic Powders for Structural and Electronic Applications. Final rept.

J. J. Ritter, and K. G. Frase. 1986, 497p Pub. in Proceedings of International Conference on Ultrastructure Processing of Ceramics, Glasses and Composites (2nd), Palm Coast, FL., March 1985, 497p 1986.

Keywords: \*Ceramics, \*Precursors, \*Titanium borides, \*Silicon carbides, \*Boron carbides, Barium titanates, Aluminum oxide, Tantalum compounds, Alcoholates, Synthesis(Chemistry), Low temperature, Yttrium compounds, Metals, Reprints.

Low temperature chemical routes to ceramic powders have received considerable attention within recent years. A novel, low temperature approach to TiB2, SiC and B4C ceramics is described as well as studies on alkoxide routes for barium polytitanates, beta/beta'' aluminas and yttrium tantalate. The concept of controlling powder crystalline phases, phase stability and particle size through manipulation of synthesis parameters is discussed.

101.068

PB91-149112 Not available NTIS National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Ceramics Div.

In situ Measurements of Bridged Crack Interfaces in the Scanning Electron Microscope.

J. Rodel, J. F. Kelly, and B. R. Lawn. 1990, 6p Sponsored by Air Force Office of Scientific Research, Bolling AFB, DC.

Pub. in Jnl. of the American Ceramic Society 73, n11 p3313-3318 Nov 90.

Keywords: \*Ceramics, \*Crack propagation, \*Fracture mechanics, Electron microscopy, Aluminum oxide, Solid-solid interfaces, Test equipment, Crack opening displacement, Reprints, In-situ tests.

A device for in situ SEM examination of crack propagation during loading of compact tension specimens is described, with a specific demonstration on an alumina ceramic. The device facilitates direct qualitative observations of the inception and subsequent frictional pullout of grain-localized bridges at the crack interface. Quantitative data on the bridging mechanism are obtained from measurements of the crack-opening displacements behind the crack tip. The crack profile is found to be closer to linear than parabolic at the bridged interface. Deconvolution of these crack-opening data allow for an evaluation of the closure tractions operative at the crack walls within the bridging zone, and thence the R-curve.

101,069

Not available NTIS PB91-149419 National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Metallurgy Div. Comparison of Flux Dynamics in Two Samples of YBa2Cu3O7 with Different Pinning.

Final rept.

M. Turchinskaya, L. H. Bennett, L. J. Swartzendruber, A. Roitburd, C. K. Chiang, M. Hill, J. E. Blendell, and K. Sawano. 1990, 4p
Pub. in Materials Research Society Symposium Proceedings, v169 p931-934 1990.

Keywords: \*Ceramics, \*Pinning, Kinetics, Magnetization, Time dependence, Temperature, Superconductors, Reprints, \*Yttrium barium cuprates.

The kinetics of magnetization in two samples of YBa2Cu3O7 prepared by different methods, are studied. Magnetization vs. time data were obtained at various temperatures for a number of applied fields. The data display (after some short period of time) logarithmic behavior and (after a sufficiently long time) exponential behavior. The pinning parameter 'activation volume' was determined from the experimental data for both samples.

101,070

PB91-149435 Not available NTIS

#### MATERIALS SCIENCES

## Ceramics, Refractories, & Glass

National Inst. of Standards and Technology (MSEL), Boulder, CO. Fracture and Deformation Div. Mechanical Loss in a Glass-Epoxy Composite. Final rept.

M. Weller, and H. Ledbetter. 1990, 3p Sponsored by Department of Energy, Washington, DC. Office of Fusion Energy. Pub. in Jnl. of Materials Research 5, n5 p913-915 May

Keywords: \*Fiber composites, \*Epoxy matrix composites, \*Mechanical measurement, \*Glass fiber reinforced plastics, Elastic properties, Torsional stress,

Using a computer-controlled inverted torsion pendulum at frequencies near 1 Hz, the mechanical losses in a uniaxially fiber-reinforced composite were deter-mined. The composite comprised glass fibers in an epoxy-resin matrix. Three fiber contents: 0, 41, and 49 vol. % were studied. Three mechanical-loss peaks appeared: above 300 K, near 200 K, and near 130 K. They correspond closely to alpha, beta, and gamma peaks found previously in many polymers. A mechanical-loss peak for either the glass or the glass-resin interface was not seen. Between 300 and 4 K, the torsion modulus increased in the resin by a factor of 3.30 and in the 0.49 glass-epoxy by a factor of 2.37.

101.071

PB91-150037 Not available NTIS National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Ceramics Div.

Improved Analysis for Flexural Creep with Application to Sialon Ceramics.

Final rept. C. F. Chen, and T. J. Chuang. 1990, 8p

Contract DE-A105-850421569
Pub. in Jnl. of American Ceramic Society 73, n8 p2366-

2373 Aug 90.

Keywords: \*Ceramics, \*Sialon, \*Creep strength, Performance prediction, Indentation, Least squares method, Compression tests, Engines, Tension tests, Bend tests, Comparison, Reprints.

By using a statistical least-squares method to minimize the differences between predicted and measured load-point displacement rates from four-point bend specimens, power-law creep parameters for tension and compression were estimated. An alternative but simpler method of estimating power-law creep parameters from flexural creep data is also proposed. The method entails the direct measurements of steadystate creep strain rates at two stress levels by an indentation technique. Based on a closed-form solution, the power-law creep parameters could then be estimated from both the measured neutral axis locations and curvature rates. The results from these two methods compare favorably with one another, and with the simple compressive creep data. Both methods yield a high stress exponent of about 14 for tension and a stress exponent of about unity for compression. Cavitation-enhanced creep in tension and diffusional creep in compression are responsible for the asymmetric behavior

101.072

PB91-158600 Not available NTIS National Bureau of Standards (IMSE), Gaithersburg, MD. Ceramics Div.

Near Net Shape Forming of Ceramics. Final rept.

S. J. Dapkunas, and A. L. Dragoo. 1987, 13p Pub. in Proceedings of ASME Winter Annual Meeting Interdisciplinary Issues in Materials Processing and Manufacturing, Boston, MA., December 13-18, 1987, p19-31.

Keywords: \*Ceramics, Processing, Manufacturing, Intelligence, Process control, Reprints, \*Net shaping.

The widespread use of advanced ceramics requires the development of reliable, economic, reproducible manufacturing. Near net shape forming is required to achieve these manufacturing goals and the many types of these forming processing offer a variety of benefits for specific applications. Ultimately the development of intelligent processing systems is required.

101.073

PR91-158774 Not available NTIS National Bureau of Standards (IMSE), Gaithersburg, MD. Ceramics Div.

National Bureau of Standards-American Ceramic Society Phase Diagram Data Program. Final rept.

J. W. Hastie. 1987, 5p

Pub. in Proceedings of International CODATA Conference (10th), Computer Handling and Dissemination of Data, Ottawa, Canada, July 14-17, 1986, p179-183 1987

Keywords: \*Ceramics, \*Data bases, Phase diagrams, Computer graphics, Mathematical models, US NBS, Thermodynamic equilibrium, Reprints.

In recent years the National Bureau of Standards-American Ceramic Society phase diagram data pro-gram has made increased use of computers in handling and disseminating the data. Computers play a key role in many areas, such as: literature retrieval, bibliographic file development, phase diagram editing, coupled thermo-chemical-phase diagram evaluation, isothermal sectioning, multi-dimensional representa-tion, and model predictions. Preparation of hard-copy compilations of phase diagrams, together with bibliographic and critical evaluation information, is also facilitated using the computer stored data. A discussion is given of the current status and future directions of the recently expanded program.

101,074 PB91-158840 Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Building Materials Div.
Towards Computer-Based Microstructure Models

for Cement-Based Systems.

H. M. Jennings. 1987, 10p Pub. in Materials Research Society Symposium Proceedings, v85 p291-300 1987.

Keywords: \*Cements, Mathematical models, Microstructure, Software engineering, Computerized simulation, Reprints.

Aspects of a computer model for cement-based systems is described. It can incorporate separately many assumptions in the form of sub-models. Two different types of sub-model are described, one that represents average characteristics of the system and one that sums individual contributions to particular characteristics of the system. The core of the overall model is a file of numbers representing the microstructure. The file is operated on to simulate hydration and the development of bulk properties.

PB91-159277 Not available NTIS National Bureau of Standards (IMSE), Gaithersburg, MD. Ceramics Div.

Tensile Creep Behavior of Structural Ceramics. Final rent

S. M. Wiederhorn, L. Chuck, and T. J. Chuang. 1986,

Pub. in Proceedings of Automotice Technology Development Contractors' Coordination Meeting (24th), Dearborn, MI., October 27, 1986, 20p.

Keywords: \*Ceramics, Heat engines, Tension tests, Creep properties, Heat resistant materials, Silicon carbides, Fracture mechanics, Performanc prediction, Sampling, Reprints.

The paper describes an inexpensive method of studying tensile creep of ceramic materials up to tempera-tures of 1500C. The technique used self aligning test fixtures, and simple grinding procedures for specimen preparation. Results suggest that tensile testing can be carried out with almost the same ease and cost as flexural testing. Since the tensile test configuration results in a simple state of stress, data from tensile testing can be used to understand creep behavior in more complex states of mechanical loading. Following the line of reasoning, data presented in the paper are being used to predict the creep behavior and state of stress in flexural bars of siliconized, silicon carbide subjected to creep at elevated temperatures.

101,076 PB91-162321 Not available NTIS Notional Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Metallurgy Div.

Superconducting Properties of Bi2-x-yPbxSnySr2Ca2Cu3Oz.

Final rept.

N. M. Seyoum, J. M. Habib, L. H. Bennett, W. Wong-Ng, and A. J. Shapiro. 1990, 6p Pub. in Supercond. Sci. Technol. 3, p616-621 1990.

Keywords: \*High-TC superconductors, \*Ceramics, Stannates, Transition temperature, Strontium compounds, Bismuth oxides, Lead oxides, Tin oxides, Strontium oxides, Calcium oxides, Copper oxides, X ray diffraction, Electron microscopy, Magnetization, Tin additions, Lead additions, Reprints.

Two systematically processed series, Bi1.6PbxSn(0.4-x)Sr2Ca2Cu3Oz and Bi(1.9-x)PbxSn0.1Sr2Ca2Cu3Oz (where X ranges from 0 to 0.4) have been examined via magnetization measurements, x-ray diffraction and scanning electron microprobe. In addition to observing the often reported high Tc superconducting transition temperatures at 80 K (2212) and 110 K (2223), a range of well resolved transition temperatures have been found, implying the possible existence of new phases. The presence of Sn in these materials appeared to suppress the formation of the low Tc Raveau 2201 phase. Also observed was an ordered variation in the amount of flux pinning as the Sn and Pb concentrations were changed. It is suggested that Sn increases flux pinning by forming the compound Sr3Sn2O7.

101.077

PB91-175075 Not available NTIS National Inst. of Standards and Technology (IMSE),

Gaithersburg, MD. Ceramics Div.
Small-Angle-Scattering Determination of the Microstructure of Porous Silica Precursor Bodies. Final rept.

G. G. Long, S. Krueger, P. R. Jemian, D. R. Black, H. E. Burdette, J. P. Cline, and R. A. Gerhardt. 1990, 10p

Pub. in Jnl. of Applied Crystallography 23, p535-544 1990.

Keywords: \*Small angle scattering, \*Silica, \*Ceramics, X-ray analysis, Neutron scattering, Sintering, Inorganic silicates, Potassium compounds, Particle size distribution, Colloids, Microstructure, Reprints, \*Ceramic pre-

Small-angle X-ray and small-angle neutron scattering measurements were carried out on a series of porous measurements were carried out on a series of policular silica precursor (unsintered) bodies with different starting chemistries. The samples were prepared from mixtures containing 10 to 30 wt% colloidal silica sol and 90 to 70 wt% potassium silicate. Particle-size distributions were derived from the data using a maximumentropy technique. Scattering data from the porous silica samples are especially suitable for such an analysis because the colloidal particles and clusters and aggregates of these particles are verified in detail to be spherical, and the scattering instrument use for the study covered the entire range of sizes in the material and was very well calibrated. It was found that the lower the amount of colloidal silica, the broader the size distribution of the silica aggregates.

101.078

PB91-175190 Not available NTIS National Bureau of Standards (IMSE), Gaithersburg, MD. Ceramics Div.

Low Temperature Chemical Route to Precursors of Boride and Carbide Ceramic Powders. Final rept.

Pub. in Materials Research Society Symposia Proceedings, v73 p367-372 1986.

Keywords: \*Ceramics, Borides, Carbides, Low temperature, Synthesis(Chemistry), Dehalogenation, Silicon chlorides, Silanes, Boron chlorides, Binary system(Materials), Titanium compounds, Reduction(Chemistry), Particulate composites, Sintering, Reprints, \*Ceramic precursors.

The controlled reductive dehalogenation of elemental halides has been studied as a low temperature approach to boride and carbide precursors. It is shown that SiCl4 and CCl4 can be reacted with metallic sodium at 130 degrees in a non-polar solvent to give the precursor to SiC. Similar type reactions with TiCl4 and BCl3 or with BCl3 and CCl4 have produced the precursors to TiB2 and B4C respectively. This procedure has also been used to generate the precursors to the two-phase composites SiC/TiC and SiC/TiN. The method is generally applicable to any combination of elemental halides which can be reduced by alkali metals or alkali metal alloys.

101.079

PB91-175620

Not available NTIS

## Ceramics, Refractories, & Glass

National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Building Environment Div.
Summary of Low-Density Glass-Fiber Reference
Materials at NIST: 1980-1989. Final rept.

R. R. Zarr. 1991, 10p

Pub. in Jnl. of Thermal Insulation 14, p211-220 Jan 91.

Keywords: \*Thermal insulation, \*Glass fibers, \*Standards, Samples, Manmade fibers, Calibrating, Metrology, Measurement, Reprints, \*Standard reference materials, National Institute of Standards and Technolo-

The paper reviews three programs at the National Institute of Standards and Technology (NIST) that provide specimens of low-density glass-fiber insulation as reference materials. The National Voluntary Laboratory Accreditation Program (NVLAP) provides speci-mens as Proficiency Test Materials; the Standard Ref-erence Materials Program (SRMP), as Standard Reference Materials; and the Center for Building Technology (CBT), as Calibrated Transfer Specimens. The pro-grams of SRMP and CBT are summarized for the years 1980 to 1989. The paper includes a catalogue of NIST publications covering the technical development of the low-density glass-fiber insulation used in the programs of NVLAP, SRMP and CBT.

101.080 PB91-187237 Not available NTIS National Inst. of Standards and Technology (IMSE), Gaithersburg, MD. Ceramics Div. Isothermal Phase Behavior of Ag3SbS3, ZnGeP2,

Final rept S. Block, G. J. Piermarini, R. G. Munro, and E. Fuller. 1989, 12p

Pub. in Physica A 156, n1 p341-352, 15 Mar 89.

\*Isothermal \*Phase Keywords: treatment Keywords: 'Isothermal treatment, 'Phase transformations(Materials), 'Silver inorganic compounds, 'Antimonides, 'Germanides, 'Single crystals, Pressure dependence, Bulk modulus, Sulfides, Phosphides, Ceramics, Wurtzite, Sphalerite, Compressibility, Equations of state, Young modulus, Reprints.

The isothermal phase behavior as a function of pressure and the bulk moduli of Ag3SbS3, ZnGeP2, and ZnS have been determined. The respective transformation pressures observed optically with single crystals are 4.9 + or - 0.15 GPa, 20 + or - 5 GPa, and 15.0 + or - 0.2 GPa. The latter transformation pressure is for both the wurtzite and sphalerite forms of ZnS. ZnGeP2 also transforms to a second high pressure phase at approximately 32 GPa. Under hydrostatic pressure zinc sulfide shows no transformation between the wurtzite and sphalerite forms. The bulk modulus was determined using the Birch, Birch-Mur-naghan, Murnaghan, and Tait equations of state with both the entire sets of compressibility data and only the linear range. The full sets of data are not as self consistent as the linear range and are useful only for interpolation. The linear sets give more reliable values for determining physical parameters such as Young's modulus. The linear sets of compressibility values yield bulk moduli and pressure derivatives: wurtizite 80 and 3.7 GPa, sphalerite 67 and 4.8 GPa, Ag3SbS3 28 and 5.6 GPa and ZnGeP2 79 and 3.2 GPa.

101,081 PB91-189449

Not available NTIS National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Reactor Radiation Div.

Structures and Properties of New Zeolite X-Type Zincophosphate and Beryllophosphate Molecular Sieves.

Final rept

W. T. A. Harrison, T. E. Gier, K. L. Moran, J. M. Nicol, H. Eckert, and G. D. Stucky. 1991, 3p Pub. in Chemical Materials 3, n1 p27-29 1991.

Keywords: \*Zeolites, \*Molecular sieves, \*Faujasite, \*Zinc phosphates, \*Beryllium phosphates, Neutron scattering, X ray scattering, Crystal structure, Phase diagrams, Aluminum silicates, FCC lattices, Reprints.

The crystal structures and properties of two new fauiasite analogues containing zinc and phosphorus (ZnPO-X) and beryllium and phosphorus (BePO-X) as the only framework tetrahedral atoms, are reported. These phases were prepared at ambient conditions and characterized by Rietveld refinement of powder neutron data (BePO-X) and powder X-ray data (ZnPO-X). Both crystallize in the face-centered cubic space group Fd bar 3 and display 1:1 Zn/Be:P tetrahedralatom order. Extra-framework cation positions have been established and these are compared with known aluminosilicate analogues. BePO-X is stable to calcination to at least 500 C, whilst the ZnPO-X framework transfers to a new phases at 300 C. The BePO-X displays a typical zeolitic ion-exchange chemistry. These novel phases are members of a large new family of non-aluminosilicate (Zn/Be,P/AsO) molecular sieves.

101.082 PB91-189704 Not available NTIS National Inst. of Standards and Technology (IMSE), Gaithersburg, MD. Ceramics Div.

Fundamental Condition for Existence of Micro-crack Clouds in Monophase Ceramics. Final rept.

B. R. Lawn. 1991, 4p

Sponsored by Air Force Office of Scientific Research, Bolling AFB, DC.

Pub. in Jril. of the European Ceramic Society 7, p17-20

Keywords: \*Ceramics, \*Fracture mechanics, \*Polycrystals, Microcracks, Crack propagation, Grain size, Defects, Residual stress, Reprints, Microcrack clouds.

Conditions for the existence of a microcrack cloud about a primary crack front in monophase polycrystalline ceramics are examined. With the assumption that microcracks initiate from sub-facet flaws, and that these flaws scale with the grain size, an expression is derived for the cloud radius. The cloud radius diminishes rapidly with grain size, from unlimited dimensions at the critical size for spontaneous, general microcracking to sub-grain level at some fraction of the critical size. The corresponding grain-size 'window' is dependent on the flaw size but is restrictively small for typical monophase ceramics.

PB91-190082 Not available NTIS National Inst. of Standards and Technology (IMSE), Gaithersburg, MD. Ceramics Div.
Indentation Determination of Crack Growth Parameters in Gallium Arsenide.

G. S. White, S. W. Freiman, and A. M. Wilson. 1991,

Contract N00014-87-F-0007

Sponsored by Office of Naval Research, Arlington, VA Pub. in Jnl. of the American Ceramic Society 74, n2 p419-421 Feb 91.

Keywords: \*Ceramics, \*Indentation, \*Crack growth, \*Fracture mechanics, \*Gallium arsenides, Measurement, Environmental tests, Water, Acetonitrile, Mechanical properties, Reprints.

Indentation measurements of the environmentally enhanced crack growth parameter, n, in GaAs have been made in water, acetonitrile, and methanol. Reasonable agreement with n values obtained from double-cantilever-beam tests was obtained. It is concluded that the range of n values which can be measured by the indentation technique is much wider than previously observed, and is strongly dependent upon the experimental configuration employed.

PB91-194670 Not available NTIS National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Ceramics Div.

Effect of Thermochemical Treatments on the

Strength and Microstructure of SiC Fibers. Final rept.

B. A. Bender, J. S. Wallace, and D. J. Schrodt. 1991,

Sponsored by Naval Air Systems Command, Washington, DC. Pub. in Jnl. of Materials Science 26, p970-976 1991.

Keywords: \*Ceramic fibers, \*Ceramic matrix composites, \*Tensile strength, \*Silicon carbides, \*Thermoche-mical properties, Thermal cycling tests, Microstructure, Thermal degradation, Fabrication, High temperature, Carbon monoxide, Annealing, Electron microscopy, Polymers, Optical microscopy, Auger electron spectroscopy, Reprints.

The room-temperature strength of commercially available polymer-derived SiC fibers degrades during the typical high-temperature thermal cycle used in ceramic matrix composite fabrication. Substantial improvements in retained room-temperature strength for two different commercially available fibers were observed after annealing in carbon powder at temperatures up

to 1600C. Further improvements in strength were observed for both fibers when heat treated in CO atmospheres. X-ray diffraction, TEM, SEM, auger electron spectroscopy, and optical microscopy were used to characterize the microstructure and chemistry of the heat-treated fibers in order to understand better the degradation mechanisms of the fibers as well as the improved strength retention.

101.085

PB91-195628 Not available NTIS National Inst. of Standards and Technology (IMSE), Gaithersburg, MD. Ceramics Div.

Phase Equilibria of the System Strontium Oxide-Calcium Oxide-Cupric Oxide. Final rept.

R. S. Roth, C. J. Rawn, J. J. Ritter, and B. Burton.

1989, 5p Pub. in Jnl. of the American Ceramic Society 72, n8 p1545-1549 1989.

Keywords: \*Ceramics, oxides, \*Calcium oxides, diffraction \*Ceramics, \*Phase diagrams, \*Crystal \*Calcium oxides, \*Strontium oxides, Copper oxides, X-ray diffraction, Orthorhombic lattices, Solid solutions, Tetragonal lattices, Reprints.

A new phase, probably CaCuO2, stable only to 740 C was found to have an orthorhombic subcell, Cmca, a = 10.588(1), b = 2.8122(4), c  $= 6.3245(6) \times 0.1$ nm with weak diffraction spots of two superimposed larger cells, one requiring 10 times the subcell b axis, the other belonging to a monoclinic lattice (interchanging b and c) with the short axis multiplied by 6 times and beta approximately = 105.5 degrees. The ternary system at 950 C shows large regions of solid solution. Complete solid solution is observed for the series (Sr, CA)2Cu03. The compound SrCuO2 accepts Ca up to Sr0.25Ca0.75O2 and Sr14Cu24O41 extends to at least Sr7Ca7Cu24O41. A new ternary phase exists with a small homogeneity region (Ca1-xSrx)CuO2 with x approximately = 0.15. The composition (Ca0.84Sr0.16)CuO2 has a primitive tetragonal unit cell with a - 3.867(2) and c = 3.2195(2)x0.1nm.

101,086

PB91-195669 Not available NTIS National Bureau of Standards (IMSE), Gaithersburg, MD

Standardization of Advanced Ceramics.

Final rept.

S. J. Schneider, and D. R. Bradley. 1988, 7p Pub. in Advanced Ceramic Materials 3, n5 p442-448

Keywords: \*Standardization, \*Ceramics, Tests, Methodology, Terminology, Mechanical properties, Data bases, Classifications, Reliability, Nomenclature, Reprints.

Advanced Ceramics, because of the superior and multifaceted properties, are being extensively developed and brought to market as rapidly as possible. A wide spectrum of commercial standards (test methods, classification system, reference materials and data) however, are lacking, and the lack may impede further marketplace diffusion and industrial acceptance. The paper elaborates upon general Advanced Ceramics standards needs and the mechanisms and organizations by which the needs could be addressed and met. Currently, a unified classification system, along with standard terminology/nomeclature are needed to set the basis for unanimity in information transfer between designers, manufacturers and product users. Standard mechanical property behavior tests, particularly high temperature procedures, have been identified as one additional singular need as mechanical integrity and reliability are pervasive requirements for all Advanced Ceramics.

101.087

PB91-202820 Not available NTIS National Bureau of Standards (IMSE), Gaithersburg, MD. Ceramics Div.

Comparison of Creep Rupture Behavior in Tension and Bending.

Final rept.

D. F. Carroll, T. J. Chuang, and S. M. Wiederhorn.

1988, 7p Pub. in Ceramic Engineering and Science Proceedings 9, n7-8 p635-641 1988.

Keywords: \*Ceramics, \*Creep properties, \*Silicon carbides, Bend tests, Tension tests, Comparison, Rupture, Compression tests, Cavities, Failure, Service life,

#### MATERIALS SCIENCES

## Ceramics, Refractories, & Glass

Performance prediction, Stress strain relations, Reprints.

Creep-rupture data in flexure are analyzed in terms of creep-rupture data in tension, and creep data obtain in both tension and compression. Based upon a critical strain criterion for cavity coalescence, and the assumption that the failure modes in tension and flexure are the same, accurate predictions of component lifetime in flexure were made.

101,088 PB91-202838 Not available NTIS National Bureau of Standards (IMSE), Gaithersburg, MD. Ceramics Div.

High Temperature Creep Testing of Ceramics. Final rept.

D. F. Carroll, and S. M. Wiederhorn. 1988, 15p Pub. in International Jnl. of High Technology Ceramics 4, n2-4 p227-241 1988.

Keywords: \*Silicon carbides, \*Ceramics, \*High temperature tests, Creep properties, Heat resistant materials, Construction materials, Tension tests, Compression tests, Loads(Forces), US NBS, Methodology, Characterization, Binary system(Materials), Failure, Reprints.

In structural applications, materials are often subjected to complex modes of loading, simple tensile or compressive stresses being uncommon. During creep de-formation, these complex modes of loading result in time dependent stress and strain distributions because ceramics tend to creep faster in tension than in compression. Consequently, creep of ceramic materials must be characterized in both tension and in compression before any predictions can be made on how a component will behave under complex stress states. Experimental techniques currently being used at the National Bureau of Standards to characterize the creep behavior of two phase ceramic materials at high temperatures are described. Techniques for creen studies in both tension and compression are usable to temperatures of 1500 C. The reliability of the test techniques with regard to linearity of loading and stability during testing is discussed.

101,089 PB91-203489 Not available NTIS National Bureau of Standards (IMSE), Gaithersburg, MD. Ceramics Div.

Small Angle Neutron Scattering Characterization of Microporous Silica.

Final rept. G. G. Long, S. T. Krueger, and R. A. Gerhardt. 1988,

Pub. in Ceramic Transactions, v5 p171-179 1988.

Keywords: \*Small angle scattering, \*Ceramics, \*Porosity, "Silica, On-line measurement systems, Neutron scattering, Characterization, Microstructure, Densification, Heat treatment, Nondestructive tests, Reprints.

The new technique of multiple small angle neutron scattering has been used to study the densification of microporous silica as a function of thermal processing. One of the advantages of small angle neutron scattering is that all of the scatterers, which in this case are pores within ceramic bodies, are measured whether they are open or closed, to yield a statistically signifi-cant determination of microstructure morphology. Furthermore, the neutron scattering techniques are nondestructive, and the time scale of data collection has been reduced, offering future possibilities for in situ measurements of microstructure evolution during processing

101,090 PB91-203786 Not available NTIS National Bureau of Standards (IMSE), Gaithersburg,

MD. Reactor Radiation Div.

Refinement of the Structure of Beta'-MoO3. Final rept.

J. B. Parise, E. M. McCarron, A. W. Sleight, and E. Prince. 1988, 4p Pub. in Materials Science Forum 27-28, p85-88 1988.

Keywords: \*Crystal structure, \*Molybdenum oxides, Rhenium oxides, Neutron diffraction, Monoclinic lat-tices, Tungsten oxides, Deuteration, Labelled com-

pounds, Oxidation, Instability, Reprints.

The structure of beta'-MoO3, a new modification of MoO3, is closely related to the structure of ReO3 and has been refined using high resolution neutron powder diffraction data and the Rietveld technique. The struc-

ture is monoclinic (P2 (sub 1)/n, a=7.415(1), b=7.433(1), c=7.654(1)A, Beta =90.09(2)). Beta' - MoO3 is isostructural with the room temperature monoclinic modification of WO3 and may be derived from the deuterated intercalate (DxMoO3), also with ReO3-type structure, by heating in oxygen at 200C. The modification is structurally intermediate between the WO3-type and the thermodynamically stable alpha-MoO3.

PB91-204172 Not available NTIS National Bureau of Standards (IMSE), Gaithersburg, MD. Ceramics Div.
Creep and Reliability of Ceramic Materials at Elevated Temperatures.

S. M. Wiederhorn, T. J. Chuang, and D. F. Carroll.

1988, 14p Contract DE-AI05-85OR21569

Sponsored by Department of Energy, Oak Ridge, TN. Pub. in Proceedings of International Symposium on Fine Ceramics Arita '87, Japan, November 17-19, 1987, p117-130 1988.

Keywords: \*Ceramics, \*Heat engines, \*Heat resistant materials, \*Creep properties, \*Silicon carbides, Constitutive equations, Failure, Reliability, Fracture mechanics, Compression tests, Tension tests, Stress strain relations, Defects, Holes(Mechanics), Cavities, Bend tests, Surface properties, Methodology, Rates(Per time), Performance prediction, Reprints.

Failure at elevated temperatures in structural ceramics often occurs as a consequence of creep deformation, which results in the generation of cavities within the ceramic. With time, cavities grow and then coalesce to form the cracks that eventually are the cause of struc-tural failure. The generation of cavities not only leads to failure of structural ceramics, but also changes the constitutive relation between creep rate and applied stress, so that, as a consequence of cavitation, creep in tension is more sensitive to stress than creep in compression. The net effect of this asymmetric behavior is a time dependence in the stress distribution when components are subjected to bending moments. Methods of measuring the creep rate in ceramic materials are discussed. Creep in tension is shown to be at least 20 times that in compression for a commercial grade of reaction bonded silicon carbide. Also, bimodal creep rate curves are observed in both tension and compression. As an example of the application of the data to more complex configurations, the constitutive equations developed for this material are used to predict the stress and strain distribution and the zone of cavitation in four point-flexure bars. Experimental data on cavitation and strain are in satisfactory agreement with predictions.

101,092 PB91-236927 Not available NTIS National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Ceramics Div.

Cyclic Fatigue from Frictional Degradation at Bridging Grains in Alumina.

Final rept. S. Lathabai, J. Rodel, and B. R. Lawn. 1991, 9p Pub. in Jnl. of the American Ceramic Society 74, n6 p1340-1348 Jun 91.

Keywords: \*Ceramics, \*Aluminum oxide, \*Fatigue life, \*Tension tests, \*Grain size, \*Fracture mechanics, Cyclic loads, Friction, Microstructure, Fracture properties, Wear, Electron microscopy, Polycrystals, Reprints, Grain bridging.

Tension-tension cyclic loading tests have been conducted on a coarse-grained alumina ceramic that exhibits toughness-curve behavior by grain-interlock bridging. Fatigue effects are observed in the regions of both short cracks, using indentation flaws, and long cracks, using compact-tension specimens. A true me-chanical fatigue effect is demonstrated by running the tests below the static fatigue limit. A custom-made device for in situ observation of crack propagation in the scanning electron microscope enables us to identify bridge degradation as a cause of the fatigue process. 'Wear' debris cumulates at the sliding intergranular frictional contact points, indicating a loss of traction at the junction. The basis of a fracture mechanics model describing the effect of the frictional degradation in reducing crack-tip shielding is outlined and fitted to the data.

101,093 PB91-236935

Not available NTIS

National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Ceramics Div.
Fracture Mechanics Model for Subthreshold In-

dentation Flaws. Part 1. Equilibrium Fracture. Final rept.

S. Lathabai, J. Rodel, T. Dabbs, and B. R. Lawn. 1991, 12p

Sponsored by Office of Naval Research, Arlington, VA. Pub. in Jnl. of Materials Science 26, p2157-2168 1991.

Keywords: \*Crack propagation, \*Models, \*Silica glass, \*Fractures(Materials), Residual stress, Defects, Equilibrium, Deformation, Cracking(Fracturing), Fracture properties, Stress intensity factors, Reprints.

A fracture mechanics model for subthreshold indenta-tion flaws is described. The model describes the initi-ation and extension of a microcrack from a discrete deformation-induced shear fault (shear crack) within the contact zone. A stress-intensity factor analysis for the microcrack extension in residual-contact and applied-stress fields is used in conjunction with appropriate fracture conditions, equilibrium in Part 1 and non-equilibrium in Part II, to determine critical instability configurations. In Part I, the K-field relations are used in conjunction with the Griffith requirements for crack equilibrium in essentially inert environments to determine: (I) the critical indentation size (or load) for spontaneous radial crack pop-in from a critical shear fault under the action of residual stresses alone; (II) the inert strengths of surfaces with subthreshold or postthreshold flaws. The theory is fitted to literature data for silicate glasses. These fits are used to 'calibrate' dimensionless parameters in the fracture mechanics expressions, for later use in Part II. The universality of the analysis in its facility to predict the main features of crack initiation and propagation in residual and applied fields will be demonstrated. Special emphasis is placed on the capacity to account for the significant increase in strength (and associated scatter) observed on passing from the postthreshold to the subthreshold

101,094 PB91-237131 Not available NTIS National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Ceramics Div.

Cathodoluminescence Measurement of Strained Alumina Single Crystals.

Final rept. C. P. Ostertag, L. H. Robins, and L. P. Cook. 1991,

Pub. in Jnl. of the European Ceramic Society 7, p109-

Keywords: \*Cathodoluminescence, \*Aluminum oxide, \*Single crystals, \*Vickers hardness, \*Residual stress, Emission spectroscopy, Measurement, Electron mi-croscopy, Spectrum analysis, Stress strain relations, Annealing, Indentation, Reprints.

Alumina single crystals indented with a Vickers hardness indenter were investigated by cathodoluminescence (CL) imaging and spectroscopy in a scanning electron microscope. The spatial resolution of the CL images was approximately 0.4 micrometers. CL spec-Intages was approximately 0.4 introllifeters. CE spectra were measured with wavelength resolution of 1.0nm in the wavelength range of 200 to 900nm; in the immediate region of the ruby lines (693 nm), spectra were measured with a resolution of 0.15 nm. Stressinduced frequency shifts of the ruby lines were utilized to measure the residual stresses in the region surrounding the indentation.

PB91-237339 Not available NTIS National Bureau of Standards (IMSE), Gaithersburg, MD. Ceramics Div.

New Layered Cuprate Structure-Type,
xA'x)14Cu24O41.

Final rept. T. Siegrist, L. F. Schneemeyer, R. S. Roth, J. V. Waszczak, and S. A. Sunshine. 1988, 10p Pub. in Materials Research Bulletin 23, n10 p1429-1438 1988

Keywords: \*Ceramics, \*Semiconductors(Materials), \*Crystal structure, \*Alkaline earth metal compounds, \*Cuprates, Calcium compounds, Lanthanum compounds, Melts, Oxides, Orthorhombic lattices, Strontium compounds, Bismuth compounds, Barium compounds, Reprints.

Phases crystallizing in a new structure-type with general formula (A(1-x)A'x)14Cu24 O41 (A = alkaline earth

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metal, A' = trivalent metal) and symmetry Cccm with an extended stoichiometry range have been found in studies of the Sr-Y-Cu-O, Ba-Sr-Cu-O, Ca-Sr-Bi-Cu-O and Ca-La-Cu-O systems. Single crystal X-ray studies on several crystals grown from different alkaline earth/ metal oxide-cuprate melts reveal a common orthorhombic F-centered subcell of a=11.3A, b=13.0A and c=3.9A. Super-structure is observed in crystals, leading to a 7-fold increase of the c-axis and a change in symmetry to space group Cccm. As in Ba2YCu3O7, the Cu atoms are found as Cu-O planes and linear Cu-O chains. Due to shear in the planes, half of the Cu-O squares share edges, producing Cu-Cu zigzag chains, similar to the planes observed in CaCu2O3. In the linear Cu-O chains, the Cu-O squares share edges as well, leading to a short Cu-Cu contact of 2.75A. Experiments on ceramic samples indicate that the oxygen content is fixed and that the samples are semiconduct-

101,096 PB91-237628

Not available NTIS National Inst. of Standards and Technology (IMSE), Gaithersburg, MD. Polymers Div.

Fourier Transform Infrared Analysis of Ceramic Powders: Quantitative Determination of Alpha, Beta, and Amorphous Phases of Silicon Nitride.

T. K. Trout, R. A. Faltynek, F. E. Brinckman, and J. M. Bellama. 1989, 5p

Pub. in Jnl. of Materials Research 4, n2 p399-403

Keywords: \*Fourier transformation, \*Infrared spectroscopy, \*Ceramics, \*Quantitative analysis, \*Silicon nitrides, Compositions, Powders, Spectrum analysis, Amorphous materials, Crystal structure, Ternary systems, Phase diagrams, Reflectance, Reprints.

Fourier transform infrared spectroscopy (FT-IR) forms the basis for determining the morphological composition of mixtures containing alpha, beta, and amorphous phases of silicon nitride. The analytical technique involving multiple linear regression treatment of Kubelka-Munk absorbance values from diffuse reflectance measurements, yields specific percent composi-tion data for the amorphous phase as well as the crystalline phases in ternary mixtures of 0-1% by weight Si3N4 in potassium bromide.

101,097 PB91-237743

Not available NTIS National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Ceramics Div.

Environmentally Enhanced Fracture of Gallium Arsenide.

Final rept.

G. S. White, S. W. Freiman, and A. M. Wilson. 1989, 3p

Contract N00014-87-F-0007

Sponsored by Office of Naval Research, Arlington, VA. Pub. in Jnl. of the American Ceramic Society 72, n11 p2193-2195 Nov 89.

Keywords: \*Gallium arsenides, \*Ceramics, \*Fracture mechanics, Stress corrosion cracking, Environmental tests, Single crystals, Nitrogen, Crack propagation, Ammonia, Water, Methanol, Acetonitrile, Humidity, Re-

GaAs has been found to undergo environmentally enhanced fracture in water, acetonitrile, formanide, and methanol. In contrast, no effect on crack growth has been observed in ammonia gas or N2 gas at 50% relative humidity. These results are consistent with the model proposed by Michelske, et al. of electrostatically enhanced bond rupture. The lack of water controlled regions in ammonia or N2 gas is presently not understood.

101.098

PB92-116797 Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Chemical Engineering Science Div.

Design and Fabrication of a Miniature High-Temperature Guarded-Hot-Plate Apparatus.
Final rept.

B. J. Filla. 1990, 8p

Pub. in Proceedings of International Thermal Conductivity Conference (21st), Lexington, KY., October 15-18, 1989, p67-74 1990.

Keywords: \*Test equipment, Ceramics, Thermal conductivity, Measurement, Ceramic matrix composites, Oxidation, Corrosion, High temperature tests, Design criteria, Fabrication, Thickness, Platinum, Rhodium, Reprints. \*Hot plates, Miniaturization.

miniature guarded-hot-plate apparatus has been built to measure thermal conductivity of ceramics and ceramic composites at temperatures between 700 K and 1500 K in a neutral or mildly oxidizing atmosphere. The system is composed of a set of 7.94 cm diameter boron nitride disks supported by high-purity alumina insulation board. Thermocouple-grade platinum and platinum-rhodium wiring are used for both the heater and thermometry elements. A typical specimen examined in this apparatus is 7 cm in diameter with a thickness between 1 and 8 mm. Optimal specimen thermal conductivities fall in the range of 0.05 to 5 W/(m)(K). Design features and choice of materials used in this apparatus are discussed.

101 099

PB92-116995 Not available NTIS National Inst. of Standards and Technology (MSEL),

Gaithersburg, MD. Ceramics Div.
Test Method for Tensile Creep of Structural Ceramics Using Flexure Beams.

R. F. Krause, and T. J. Chuang. 1991, 10p Pub. in Ceramics Today - Tomorrow's Ceramics, p1865-1874 1991.

Keywords: \*Ceramics, \*Construction materials, \*Flexural strength, Creep tests, Silicon carbides, Tension tests, High temperature tests, Displacement, Loads(Forces), Compression tests, Bend tests, Sintered materials, Flexing, Beams(Supports), Reprints, Power law.

A novel method of analysis is described for evaluating the power-law parameters for tensile creep of structural ceramics at elevated temperatures. Displacement rate, invariant with time in the secondary mode of creep, is measured versus load on both compression and flexure specimens of a material. The analysis takes into account that the material behaves differently in tensile and compressive creep. The power-law parameters for compressive creep are evaluated directly from strain rate versus stress in the compression tests. Using these values for compressive creep, those for tensile creep are evaluated from displacement rate versus bending moment in the flexure tests. The compressive and tensile creep properties of the material determine the curvature and neutral-axis position in the flexure specimen under a given bending moment. The power-law parameters for creep of sintered alpha silicon carbide are evaluated to demonstrate the usefulness of the method.

101.100

PB92-117001 Not available NTIS National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Reactor Radiation Div.

Characterization of the Densification of Alumina

by Multiple Small-Angle Neutron Scattering. Final rept.

S. Krueger, G. G. Long, and R. A. Page. 1991, 9p Contracts MIPR-ARO-102-90, DE-FG05-84ER45063 Sponsored by Army Research Office, Research Trian-gle Park, NC., and Department of Energy, Washington, DC.

Pub. in Acta Crystollagraphica A47, p282-290 1991.

Keywords: \*Aluminum oxides, \*Porosity, Neutron scattering, Ceramics, Small angle scattering, Sintering, Microstructure, Reprints, Pore size.

Multiple small-angle neutron scattering was used to follow the evolution of the pore-size distribution in alpha-Al2O3 through the intermediate and final stages of sintering. The new technique enables the study of microstructure in the 0.08-10 micrometers size regime, which is the size range of importance for many materials systems, without needing to increase the resolution of currently available small-angle scattering instruments. The microstructure evolution results indicate a nearly constant effective pore radius for the alumina throughout the intermediate sintering stage, ranging from 0.19 micrometers at 54% of theoretical density to 0.17 micrometers at 79% dense. As the alumina densifies further, there is a transition region after which the effective pore radius grows rapidly to greater than or equal to 0.6 micrometers at 97.5% dense.

101,101

PB92-117043 Not available NTIS National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Ceramics Div.

Effect of Green Density and the Role of Magnesium Oxide Additive on the Densification of Alumina Measured by Small-Angle Neutron Scattering.

G. G. Long, S. Krueger, and R. A. Page. 1991, 7p Pub. in Jnl. of the American Ceramic Society 74, n7 p1578-1584 Jul 91.

Keywords: \*Aluminum oxides, \*Densification, \*Ceramics, Neutron scattering, Small angle scattering, Density, Green strength, Sintering, Magnesium oxides, Measurement, Additives, Porosity, Microstructure, Characterization, Reprints.

Small-angle neutron scattering measurements were used to examine the effect of green density and the role of MgO additive on the evolution of the porous microstructure of alumina during intermediate- and final-stage sintering. It was found that the initial connectivity in the green state plays a dominant role in establishing the channel diameters during the intermediate stage of sintering, and contributes also to determining the onset density at which the final stage of sintering begins. The role of MgO as a sintering aid lies, at least in part, in prolonging the stability of intermediatestage sintering such that the body achieves greater density before the transition to final-stage sintering after which isolated pores are formed.

101,102

PB92-117357 Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Chemical Engineering Science Div. Apparent Thermal Conductivity of Fumed-Silica Standard Reference Materials.

Final rept. D. R. Smith. 1990, 16p Contract ORNL/IA-21428

Sponsored by Oak Ridge National Lab., TN. Pub. in Proceedings of International Thermal Conductivity Conference (21st), Lexington, KY., October 15-18, 1989, p261-276 1990.

Keywords: \*Vapor deposition, \*Thermal conductivity, 'Silica, \*Insulating boards, Fumes, Measurement, Microporosity, Temperature dependence, Atmospheric pressure, Pressure dependence, Density, Statistical analysis, Moisture content, Reprints, \*Fumed silica, Standard reference materials, Hot plates.

Measurements of apparent thermal conductivity of microporous fumed-silica insulation board (MFS) are reported here for mean specimen temperatures ranging from 318 to 733 K (45 to 460 C) and environmental air pressures from 83.5 kPa (626 Torr) down to 27 kPa (200 Torr). Apparent conductivity is correlated with temperature, pressure, and density; the correlation obtained represents the data within a standard deviation of 0.68 percent. MFS with a density of 300 kg/cu m and at an ambient pressure of 83 kPa has an apparent thermal conductivity of 19.8 mW/(m K) at 300 K. It is suitable for use as a standard reference material of very low conductivity from 297 to 733 K (24 to 460 C). Adsorbed moisture within this material must be driven off by prolonged heating at 110 C before its conductivity is measured. Great care in handling MFS is necessary because of its fragility.

101,103

PB92-117449 Not available NTIS National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Ceramics Div. Effect of Surface Forces on Subcritical Crack

Growth in Glass.

Final rept. S. M. Wiederhorn, and E. R. Fuller. 1989, 4p Pub. in Jnl. of the American Ceramic Society 72, n2 p248-251 Feb 89.

Keywords: \*Surface forces, \*Crack propagation, Silica glass, Fracture mechanics, Aqueous solutions, Stress intensity factors, pH, Surface chemistry, Re-

Data on the growth of cracks tested in aqueous solutions were interpreted in terms of surface force theory. For applied stress intensity factors greater than 0.25 MPa (m(sup 0.5)), the position and the slope of the curves and their dependence on pH and ion concentration can be explained in terms of surface force theory, provided these forces are of a magnitude and range that are representative of those involved in the cohesive bonding of solids. Weaker forces, such as structural, double-layer, or dispersion forces, have little

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effect on crack growth in silica glass for  $K(sub\ 1) > 0.25 MPa (m(sup\ 0.5))$ .

101,104

PB92-126507 PC A09/MF A02 National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Ceramics Div. Ceramics: Technical Activities 1991. (NAS-NRC As-

sessment Panel, February 13-14, 1992).

Annual rept. S. W. Freiman. Feb 92, 176p NISTIR-4694 See also PB91-132233

Keywords: \*Research projects, \*Ceramics, Standards, Materials, Mechanical properties, Processing, Superconductors, Microstructure, Synchrotron radiation, bology, Patents, Vapor deposition, Databases, Photonic materials, Optoelectronic materials, Advanced ceramics, Ferroelectric oxide films, High temperature superconductors.

In 1991, the Ceramics Division continued its program of standards development, data generation and evaluation, and research focused on the characterization and understanding of material behavior. The research program focuses on the critical issues which control the implementation of advanced ceramics and is developed through internal assessment and consultation with representatives from ceramic industries and academia. Some areas of research were: ferroelectric oxide films, glass compositions, advanced ceramics, powder processing, modelling and superconductivity.

101.105

PB92-126564 PC A05/MF A01 National Inst. of Standards and Technology (EEEL), Boulder, CO. Electromagnetic Technology Div. High-Temperature Superconductivity: Abstracts of NIST Publications, 1987-1991.

M. E. DeWeese. Nov 91, 93p NIST/SP-826 Also available from Supt. of Docs. Supersedes PB89-148340

Keywords: \*Ceramics, \*Superconductivity, \*Abstracts, Bismuth, Standards, Thallium, Yttrium, High temperature tests, Thin films, X ray diffraction, Crystal defects, Phase transformations.

The report is a collection of abstracts from 243 papers published between March 1987 and August 1991 covering various aspects of superconductivity research. The work of nine divisions of the National Institute of Standards and Technology (formerly the National Bureau of Standards) in both Boulder, Colorado, and Gaithersburg, Maryland, is represented.

#### Coatings, Colorants, & Finishes

PC A03/MF A01 AD-A243 095/7 National Inst. of Standards and Technology, Gaithersburg, MD.

Chemical Vapor Deposited Diamond.

Technical rept. A. Feldman, E. N. Farabaugh, and L. H. Robins. 27 Sep 91, 50p

Contract N00014-90-F-0011

Keywords: Chemical reactions, Chemicals, Coefficients, Deposition, \*Diamonds, Diffusion, Electrical resistance, Far infrared radiation, Frequency, Friction, Measurement, Modulus of elasticity, Optics, Perme-ability, Room temperature, Single crystals, Thermal conductivity, Transparencies, \*Vapor deposition, conductivity, Chemical vapor deposition.

There is considerable interest in using diamond for numerous applications because of the development of methods that allow for the deposition of diamond by chemical vapor deposition (CVD) techniques over large areas. The interest in new applications for diamond rests on combinations of superior properties that diamond possesses. These extreme properties, which are based on measurements in bulk single crystal diamond, include greatest hardness, highest elastic moduli, and highest thermal conductivity at room temperature of any material. Other important properties include optical transparency over an extensive wavelength range from the ultraviolet through the far infrared, high electrical resistivity, dopability to be a semiconductor, low permeability to diffusion, chemical inertness, and low coefficient of friction.

101,107 PB91-167395 PC A05/MF A01 National Inst. of Standards and Technology (MSEL), Gaithersburg, MD.

U.S. Assessment of the New Diamond Technology in Japan.

Special pub. (Final). A. Feldman, and L. H. Schwartz. Jan 91, 100p NIST/

Also available from Supt. of Docs. as SN003-003-03067-8

Keywords: \*Diamonds, \*Vapor deposited coatings, \*Chemical vapor deposition, \*Japan, Etching, Abrasives, Polishing, Reviews, Epitaxy, Ion implantation, Laser cutting, Cutting tools, Heat sinks, Electro-optics, Optical materials, Research projects, Lithography, International cooperation, Boron nitrides, Ceramics, Industrial engineering.

The assessment of Japanese diamond technology was undertaken at the request of the joint committees for implementation of the 1988 United States-Japan Agreement on Cooperation in Research and Development in Science and Technology under the auspices of the Committee on Materials, Office of Science and Technology Policy. The purposes of the study were to assess the level of scientific activity, areas of intended commercialization, progress in commercialization, the role of the Japanese government in assisting industry to exploit the new diamond technology, and the relative positions of Japan and the U.S. in all aspects of synthesized diamond technology. Japanese efforts were chosen for assessment because Japan is the apparent world leader in the drive for commercialization of the technology. The principal focus of the study was diamond produced by chemical vapor deposition, with a peripheral investigation of cubic boron nitride and diamond-like carbon. Based on the assessment, a set of conclusions and recommendations is presented. The assessment is based on site visits in Japan between May 28 and June 5, 1990.

101,108 PB91-195248

Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Building Materials Div.
Fourier Transform Infrared Spectroscopic Studies

of the Degradation of One-Component Polyether Polyurethane Protective Coatings on Steel. Final rept.

T. Nguyen, and W. E. Byrd. 1988, 20p Pub. in Proceedings of FATIPEC Congress (19th), v3

p255-274 1988.

Keywords: \*Protective coatings, \*Steels, \*Polyurethanes, \*Polyethers, \*Corrosion mechanisms, Polymers, Construction materials, Fourier transformation, Infrared spectra, Degradation, Time dependence, Brittle materials, Dissociation, Reprints.

The degradation of one-component polyether polyurethane coatings on steel in corrosive environments was investigated using reflection/absorption Fourier transform infrared spectroscopy (FTIR-RA). Coatings of about 2 micrometers were applied uniformly to the me-chanically polished (0.25 micrometer) cold-rolled steel substrates using a spin coater. After curing at room conditions, the coated specimens were exposed to an aerated 40C and 80% RH environment. The studies showed that considerable chemical changes occurred in the structure of the coating after 8 months exposure to the exposure environment. Besides changes in the intensities of the amino, carbonyl and isocyanate groups, some of the hydrogen bonded amino groups also become dissociated. Exposure in the environment also results in extensive brittleness and crazing in the polyurethane coatings. The competitive formation and degradation reactions of various chemical groups in polyurethane during exposure will also be discussed.

PB91-203729 Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Building Materials Div.

Characterization of Epoxide Coatings on Steel by Reflection/Absorption Fourier Transform Infrared Spectroscopy: Quantitative Study.

Final rept.

Final rept.
T. Nguyen, W. E. Byrd, and D. P. Bentz. 1988, 18p
See also PB88-175518.
Pub. in Proceedings of FATIPEC Congress (19th), v2

Keywords: \*Polymeric films, \*Epoxy resins, \*Steels, \*Coatings(Materials), Thickness, Characterization, Thin films, Spectrum analysis, Infrared spectra, Calculation methods, Fourier transformation, Theories, Substrates, Absorptivity, Reflection, Transmission, Comparative evaluation, Reprints.

The study examines, both theoretically and experimentally, the effects of film thickness and angle of incidence on band shape intensities of an epoxy coating on a steel substrate. Crosslinked epoxy films between 10nm and 25 micrometers were uniformly spin coated on 25x25mm, mechanically polished (0.25 micrometers), cold-rolled steel samples. The most intense band of an epoxy coating, the 1510 1/cm band, was used for the study. There is a good linearity between band intensity and film thickness up to about 200nm; above that it deviates form Beer-Lambert law. Above 250nm, the theory underestimates the intensity and in this range a power law expression is more useful to estimate film thickness from the peak height of a FTIR-RA spectrum. For thin films (100nm), the theory agrees very well with experimental results on the relationship between band intensity and angle of incidence. How-ever, for thick films the theory underestimates the intensity at low angles of incidence and overestimates at high angles of incidence, particularly in the micrometer thickness range. There are certainly some differences between the spectrum of an epoxy on steel substrate obtained by the FTIR-RA technique and that of a film on NaCl obtained by the transmission technique. These differences become quite pronounced in thick

101 110

Not available NTIS PB91-204073 National Inst. of Standards and Technology (IMSE), Gaithersburg, MD. Metallurgy Div Magnetic Properties of Iron/Silica Gel Nanocom-

posites. Final rept.

R. D. Shuli, J. J. Ritter, A. J. Shapiro, L. J. Swartzendruber, and L. H. Bennett. 1989, 6p Pub. in Materials Research Society Symposium Proceedings, v132 p179-184 1989.

Keywords: \*Silica gel, \*Iron, \*Particulate composites, \*Magnetic properties, \*Paramagnetic materials, Matrix materials, Spin glass, Homogeneous mixtures, X-ray diffraction, Porosity, Particle size, Mossbauer effect, Spectrum analysis, Heating, Temperature depend-ence, Hydrogen, Ammonia, Superparamagnetism, Re-prints, \*Nanocomposites.

Homogeneous gelled composites of iron and silica containing 5-30 wt. % Fe have been prepared by low temperature polymerization of aqueous solutions of ferric nitrate, tetraethoxysilane, and ethanol (with an HF catalyst). X-ray diffraction data indicated that these bulk materials are comprised of nanometer-sized regions of iron compounds embedded in a silica gel matrix. Scanning electron microscopy observations show that this matrix is characterized by the presence of many interconnected pores and that the size of these pores is related to the particle size of the Fe-containing regions. The paramagnetic nature of these materials at room temperature, as well as small size of the iron-containing regions, is indicated by the appearance in many of the sample of only a high intensity central doublet in the (57) Fe Mossbauer spectra. The Mossbauer effect data indicated that the form of the iron can be changed by a subsequent treatment in an atmosphere of ammonia or hydrogen at elevated temperatures. In addition, magnetic susceptibility measurements indicated that the hydrogen treated material becomes a spin glass at low temperatures.

PB91-237669 Not available NTIS National Inst. of Standards and Technology (MSEL), Variations in the Practice of Ceramic Technology

(WSE2),

Variations in the Practice of Ceramic Technology

in Different Cultures: A Comparison of Korean and Chinese Celadon Glazes.

Final rept.

P. B. Vandiver, L. A. Cort, and C. A. Handwerker. 1989, 42p

Pub. in Ceram. Civiliz. 4, p347-388 1989.

Keywords: \*Ceramic glazing, \*Archaeological specimens, \*Glazed ware, \*Porcelain, Korea, China, Technology transfer, Comparison, Reprints, \*Celadon.

Korean celadon glazes remained quite constant in visual appearance and technology during the Koryo

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dynasty (A.D. 918-1392), the result of a conservative craft workshop tradition which supplied green-glazed wares for the court, and they changed very little during the early Choson dynasty (fifteenth century) when they became a popular ware. The technological feat is contrasted with the diversity in visual appearance and ceramic technology found in Chinese celadons. The potential interactions of these traditions are explored.

101.112 PB92-116813 Not available NTIS National Bureau of Standards (IMSE), Gaithersburg, MD. Ceramics Div. Heat Conductivity of Oxide Coatings by Photother-

mal Radiometry between 293 and 1173 K.

Final rept. H. P. R. Frederikse, and X. T. Ying. 1988, 4p Pub. in Applied Optics 27, n22 p4672-4675 1988.

\*Coatings(Materials), \*Metal oxides, \*Ceramics, Photothermal conversion, Nondestructive tests, Substrates, Radiometers, Reprints, Thermal waves.

Optical generation and optical detection of thermal waves are being used to determine the thermal properties of oxide coatings on metal substrates.

#### **Composite Materials**

AD-A231 778/2 PC A03/MF A01 National Inst. of Standards and Technology (IMSE), Gaithersburg, MD. Metallurgy Div. Influence of Water on the Mechanical Properties of

a Glass-Epoxy Matrix Composite. Technical rept. 1 Feb 89-1 Feb 91. M. R. Stoudt, E. Escalante, and R. E. Ricker. 12 Feb

Contract N00014-89-F-0072

Keywords: Absorption, Degradation, Desorption, Epoxy compounds, Glass, High pressure, Intervals, Matrix materials, Mechanical properties. Orientation(Direction), Pressure, Sampling, Water. Weight, \*Composite materials.

The influence of exposure to water at ambient pressure and at an elevated pressure on the mechanical properties of a glass fiber epoxy matrix composite was investigated. The mechanical properties of three orientations of the composite were determined in the dry condition, after exposure to water at ambient pressure and after exposure to water at 5.9 MPa. Then, to determine the mechanism of the observed degradation, the mechanical properties of samples exposed at the two pressures were determined after the absorbed water was removed. The rate and extent of water absorption and desorption was evaluated by measuring the weight change at periodic intervals.

AD-A239 509/3 AD-A239 509/3 PC A03/MF A01 National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Corrosion Group. Influence of Moisture and Pressure on the Me-

chanical Properties of a Glass-Epoxy Matrix Composite and a Graphite-Epoxy Matrix Composite.

Technical rept. no. 2, 1 Feb 89-1 Feb 91.

M. R. Stoudt, E. Escalante, and R. E. Ricker. Jul 91,

30p

Contract N00014-89-F-0072

Keywords: Absorption, \*Composite materials, Degradation, Desorption, Dry materials, Epoxy compounds, Exposure(General), Fibers, Graphited materials, High pressure, Intervals, Matrix materials, Mechanical properties, Moisture, Orientation(Direction), Pressure, Sampling, Strength(Mechanics), Water, Weight, Wet strength, Yield strength, \*Glass, \*Graphite epoxy composites, \*Epoxy composites, Hydrostatic pressure, posites, \*Epoxy composites, Hydrostatic pressure, Water absorption, Moisture content, Fiber reinforced composites, Polymers, Plasticity, Glass fibers.

The influence of exposure to water at ambient pressure and at elevated pressure was evaluated on the mechanical properties of a glass fiber-epoxy matrix composite and a graphite fiber-epoxy matrix composite. The mechanical properties of three different fiber orientations for each material were measured in the dry condition, after exposure to water at ambient pressure and after exposure to water at 5.9 MPa. In order to determine if the observed degradation was permanent, the mechanical properties were also measured after the absorbed water was removed. During exposure, the rate and extent of water absorption and desorption was evaluated by measuring the weight change at periodic intervals. Substantial reductions in the vield strength and ultimate strength were observed in the wet condition for the glass epoxy samples at both pressures, while the strength of the graphite epoxy composite was found to be insensitive to the water exposure. The wet strength of the glass epoxy composite was found to be independent of water pressure during absorption and upon desorption, complete recovery of the dry strength was demonstrated. Evidence of compression-induced failure was observed for the graphite-epoxy composite in the wet condition.

701,115 PB91-132191 PC A05/MF A01 National Inst. of Standards and Technology (MSEL), Gaithersburg, MD.

Polymer Composite Processing. Industry Workshop (2nd). Held at Gaithersburg, Maryland on May

C. Johnson, S. S. Chang, and D. Hunston. Dec 90, 87p NISTIR-4461 See also PB88-179882.

Keywords: \*Thermosetting resins, \*Composite materials, \*Fiber composites, \*Meetings, Processing, Molding techniques, Pressing(Forming), Filament winding, Preimpregnating, Standards, Heat transfer, Delaminating, Creep properties, Fatigue life, Environmental tests, Microstructure, \*Polymer matrix composites, \*Resin matrix composites, Prepregs, Solid-Solid interfaces.

Industry representatives identified the most important processing methods, and scientific and technical barriers to improved polymer composite processing. Two processing methods were selected as most important: pressure molding and liquid molding. Seven scientific and technical barriers to the full exploitation of these processing methods were identified. The three highest priority items are the need to understand and control resin flow and fiber orientation, to develop process monitoring sensors for on-line control, and to understand and control the fiber-matrix interface. The remaining areas where there is a need for improvement are data validation and testing standards, determination and control of morphology, surface quality and dimensional stability, and understanding of heat flow. The Workshop also identified and prioritized eight technologies that complement processing and are important for the future. The three highest ranked items were fiber placement, new methods to prepare prepreg, and joining. The remaining items are preform preparation, recycling, environmental safety, tooling, and alternate sources of energy. The majority of people at the Workshop felt that thermosets were still the dominant resin system in most applications. The Workshop also selected seven performance issues that they felt were critical for the future: impact, environmental attack, delamination, dimensional changes, thermal stability, fatigue, and creep.

101,116 PB91-147090 Not available NTIS National Inst. of Standards and Technology (MSEL),

Gaithersburg, MD. Polymers Div.
Effect of Logarithmic Singularity on the Free Edge
Stress Intensity Factor of Composite Laminates. Final rept

M. Y. M. Chiang, and H. K. Stolarsky. 1990, 14p Pub. in Proceedings of Technical Conference on Composite Materials (5th), East Lansing, Ml., June 11-14, 1990, p336-349.

Keywords: \*Laminates, \*Stress intensity factors, Composite materials, Singularity, Reprints.

The study explains the relative importance of two types of stress singularities (r(sup delta) and log r), which may occur at the free edge of laminates. The r(sup delta) singularity and log r singularity are merged to describe the edge effects of composite laminates. A combination of asymptotic analysis, which gives the strength of the singularity, and enriched finite element method (global/local technique) is used to solve a complete boundary value problem. The numerical results have been obtained for three different composite laminates: (45 deg/-45 deg) laminate, (90 deg/15 deg) laminate and (-15 deg/75 deg) laminate. It is concluded that the inclusion of the additional weaker singularity (log r) may significantly change the value of the

stress intensity factor based on consideration of the strong singularity (r(sup delta)) alone.

101,117

PB91-159178 Not available NTIS National Inst. of Standards and Technology (MSEL), Spin Glass Magnetic Behavior of Iron/Silica Gel

Nanocomposites.

Final rept. R. D. Shull, and J. J. Ritter. 1990, 6p

Pub. in Materials Research Society Symposium Proceedings, v195 p435-440 1990.

Keywords: \*Composite materials, \*Iron compounds, \*Silica gel, \*Spin glass, \*Polymers, Magnetic properties, Paramagnetic materials, Magnetic permeability, Measurement, Cryogenics, Anisotropy, Ferromagnetic materials, X-ray diffraction, Mossbauer effect, Electron microscopy, Reprints, \*Nanocomposites.

Homogeneous gelled composites of iron and silica containing 5.40 wt.%Fe prepared by low temperature polymerization of aqueous solutions of ferric nitrate, tetraethoxysilane, and ethanol (with an HF catalyst) were heated to 380 C in the presence of hydrogen gas. X-ray diffraction and Mossbauer effect measurements, and transmission electron microscope (TEM) observations show these materials are comprised of nanometer-sized regions of iron compounds embedded in a silica gel matrix. Magnetic susceptibility data indicate the materials became either superparamagnetic or ferromagnetic at room temperature. On cooling, the magnetization data furthermore show that the hydrogenated materials containing 11-30%Fe become magnetic spin glasses at temperatures less than 30K. Magnetic history effects are observed in addition to displaced hysteresis loops below their spin freezing temperatures (Tf). For field-cooled materials at 10 K, the displacement of the hysteresis loops along the field axis indicates the presence of a unidirectional anisotropy which decreases with the cooling field. Both superparamagnetic-to-spin glass and ferromagnetic-to-spin glass transitions are observed in these nanocomposites. If varies with the Fe content from approximately 30 K for the 11%Fe nanocomposite to approximately 10 K for a content near 33%Fe.

PB91-162180 Not available NTIS National Inst. of Standards and Technology (IMSE), Boulder, CO. Fracture and Deformation Div.

Mechanical Properties of Alumina-Peek Unidirec-

tional Composite: Compression, Shear, and Tension.

Final rept.

R. D. Kriz, and J. D. McColskey. 1990, 7p Sponsored by National Aeronautics and Space Administration, Moffett Field, CA. Ames Research Center. Pub. in Advances in Cryogenic Engineering (Materials) 36, p921-927 1990.

Keywords: \*Aluminum oxide, \*Fiber composites, \*Ceramic matrix composites, Cryogenics, Compression tests, Low temperature, Thermoplastics, Fracture strength, Fatigue, Tension tests, Shear tests, Peek,

A new Al2O3 (alumina) fiber composite with high strain to failure was fabricated with a thermal plastic PEEK (poly-ether-ether-ketone). The Al2O3-PEEK composite shows a marked improvement over thermally setting composite in that it absorbs 150 percent more elastic strain energy at 76 K than at room temperature. This increase in fracture toughness at low tempera-tures can provide improved fatigue performance for thermal isolation straps at low temperature. Other mechanical property results suggest improvements for applications where graphite-epoxy materials are presently being used at low temperatures and where light weight is not a critical issue.

101.119

PB91-174656 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Ionizing Radiation Div.

Emissivity of Aluminized Mylar.

Final rept.

S. R. Domen. 1991, 3p Pub. in Radiation Physics and Chemistry 37, n2 p199-201 1991

Keywords: \*Thermal insulation, \*Polyethylene terephthalate, \*Aluminum coatings, Calorimeters, Com-

#### **MATERIALS SCIENCES**

## **Composite Materials**

posite materials, Plastics, Graphite, Thermal emission, Polymeric films, Metallizing, Reprints.

Commercially-available aluminized Mylar, 6 micrometers thick, is a useful material for reducing heat losses by thermal radiation in some calorimeters, such as those constructed of graphite or A-150 plastic. The present experiment shows that clean aluminized layers have a thermal emissivity near 0.044.

101.120

PB91-174946 Not available NTIS National Inst. of Standards and Technology (MSEL), Boulder, CO. Fracture and Deformation Div. Numerical Simulation and Visualization Models of

Stress Wave Propagation Graphite/Epoxy Com-

posites. Final rept.

Pub. in Review of Progress in Quantitative Nondestructive Evaluation, v9 p125-132 1990.

Keywords: \*Stress waves, \*Wave propagation, \*Computerized simulation, \*Finite difference method, \*Composite materials, Nondestructive tests, Supercomputers, Finite element method, Elastic waves, Wave phases, Reflection, Reprints.

Based on previous results by finite elements the authors have extended their studies to include a fourth order splitting finite difference scheme of MacCor-mack. The finite difference method has allowed the authors to solve much larger problems. With a finite element method a mesh with 16458 degrees of freedom was solved in 2.2 hours on the NIST Cyber 205. With the finite difference scheme a mesh with 221502 degrees of freedom was solved in 70 seconds without using the full memory capacity of the Cyber 205. With this improved numerical method more accurate stress wave propagation simulations were possible. The authors studied some interesting phenomena observed in previous studies where the mesh was too coarse to In previous studies where the mesh was too coarse to conclude meaningful results. They studied the reflection of a single pulse in an off-axis unidirectional graphite/epoxy composite where the large deviation angle of the propagating wave resulted in a short lived sufface wave shift of the reflected wave. A colored movie of this phenomena shows L, qL, qt and t modes and other physical phenomena not predicted by simple plane-wave theory.

101.121

PB91-185116 PC A09/MF A01 National Inst. of Standards and Technology (MSEL), Boulder, CO. Materials Reliability Div.

Effect of a Free Surface on Stress Distribution in a Bimaterial Composite.

Special pub. (Final). V. K. Tewary, and R. D. Kriz. Mar 91, 186p NIST/SP-802

Also available from Supt. of Docs.

\*Stress analysis, surfaces(Crystallography), \*Composite materials, Binary system(Materials), Greens function, Elastic properties, Loads(Forces), Grain boundaries, Equations, Solid-solid interfaces, Plane strain, Free edge

The paper is in two parts. In Part I, the SI Green's function is calculated and applied to plane-strain problems in cubic solids. In Part II, an extension of the Green's function method to the generalized-plane-strain prob-lem is described, which enables the calculation of the elastic response of a solid to a prescribed out-of-plane strain. It is applied to calculate the stress distribution in a composite solid subjected to an out-of-plane load. The final results are in the form of an analytical closed integral representation which can be calculated numerically as well as analytically. The analytical evalua-tion of the integral by using the contour integration method gives the result in the form of a series. The series contains singular as well as non-singular terms. In general, it is difficult to ascertain the convergence of the series representation. The analytical series representation can be used to identify precisely the nature and the weight of each singularity in the stress distribu-

101,122

PB91-187336 Not available NTIS National Inst. of Standards and Technology (IMSE), Gaithersburg, MD. Polymers Div.

Interlaminar Shear Fracture of Laminated Composites. Final rept.

H. Chai. 1990, 15p Pub. in International Jnl. of Fracture 43, p117-131

Keywords: \*Resin matrix composites, \*Composite materials, "Fracture mechanics, Fracture strength, Electron microscopy, Surface energy, Adhesion, Plasticity, Deformation, Performance prediction, Reprints, Interlaminar shear.

The interlaminar fracture toughness in mode II and mode III of a number of advanced composites was studied using beam type test specimens and scanning electron microscopy. Special emphasis was placed on elucidating the material aspects of the fracture proc-ess and on quantifying the effect of matrix on fracture energy. The fracture energy in mode II was independ-ent of crack extension while that for mode III exhibited a rather probabilistic 'resistance' behavior that was at-tributed to the effect of fiber bridging. The initiation fracture energy, considered here the true measure of G(IIIc), coincided with G(IIc). For either mode, the interlaminar region ahead of the crack tip exhibited considerable plastic deformations, the severity that is be-lieved to control the laminate toughness. The interlaminar fracture energy in shear, hereby denoted as G(sc) (=G(IIc)=G(IIIc)), was accurately predicted from a straightforward adhesive joint fracture test provided the adhesive thickness coincide with the thickness of the interlaminar resin layer.

PB91-194878 Not available NTIS National Inst. of Standards and Technology (MSEL), Boulder, CO. Fracture and Deformation Div. Elastic Constants of Fiber-Reinforced Compos-

ites: A Fresh Measurement Approach. Final rept.

Pub. in Proceedings of Ultrasonics Symposium, Honolulu, Hl., December 4-7, 1990, p1267-1269.

Keywords: \*Fiber composites, \*Elastic properties, \*Metal matrix composites, \*Graphite composites, \*Ultrasonic tests, Measurement, Methodology, Magnesium, Reprints.

Composites reinforced with uniaxial fibers often possess transverse-isotropic symmetry and, therefore, five independent elastic constants: C11, C33, C44, C66, C13. (X3 is the fiber direction, X1 the plate-normal direction.) Measurements on a single speci-men along principal axes give all the Cij except C13. To get C13, the usual approach is to propagate waves in nonprincipal directions such as (110). A fresh approach is proposed that requires measurements only along principal directions: <100>. The approach also avoids the thin-plate problem, where measuring C22 and C33 may be difficult. In the new approach, a pulse-echo (megahertz-frequency) method is used to meas-ure C11, C44, C66. (All three involve waves propagating along X1, through the plate.) A resonance (kilo-hertz-frequency) method is used to measure two elastic compliances: S11 and S33, S44, and S12 come from simple formulas containing C44 and C66. S13 comes from a relatively simple formula containing S11, S12, S33, and C11. The new approach is applied to a graphite-magnesium composite.

PB91-195362 Not available NTIS National Inst. of Standards and Technology (IMSE), Gaithersburg, MD. Ceramics Div. Reduction in Sintering Damage of Fiber Rein-

forced Composites.

Final rept. C. P. Ostertag. 1990, 8p Pub. in Ceramic Transactions 7, p745-752 1990.

Keywords: \*Sintering, \*Fiber composites, \*Ceramic matrix composites, \*Fracture mechanics, \*Residual stress, Stress tests, Crack propagation, Loads(Forces), Compression tests, Processing, Reprints.

Sintering of fiber reinforced composites results in the creation of residual stresses. Previous experiments revealed that these stresses initiate in the early stage of sintering usually during the heating cycle, and may be responsible for the sintering damage observed in fiber-reinforced composites. Processing techniques were developed to reduce stress generation during the heating cycle by applying uniaxial compressive

stresses in the range of 0.5 MPa to 2.3 MPa to the green composites and compare the results with com-posites under no load. The application of a compressive load increases the matrix density and hence, after the load is removed, the critical stress necessary for crack formation is increased. No sintering damage such as crack formation was observed after the composites were subjected to a compressive stress of 1.5 МРа.

101.125

PB91-202952 Not available NTIS National Bureau of Standards (IMSE), Gaithersburg, MD. Ceramics Div.

Effect of Thermal Expansion Mismatch on Fiber Pull-Out in Glass Matrix Composites.

Final rept.

U. V. Deshmukh, A. Kanei, S. W. Freiman, and D. C. Cranmer. 1988, 6p Pub. in Materials Research Society Symposium Pro-

ceedings, v120 p253-258 1988.

Keywords: \*Interfacial tension, \*Thermal expansion, \*Fiber composites, \*Ceramic fibers, \*Glass, \*Matrix materials, Carbon fibers, Silicon carbides, Sliding friction, Borosilicate glass, Silica glass, Alkali glass, Moisture content, Shear strength, Stress tests, Wetting, Reprints, Fiber pull-out.

Single fiber pull-out tests can be used to directly measure the fiber-matrix interfacial shear stress in glass matrix composites. The system under investigation consisted of a soda-lime-silica glass matrix containing SiC monofilaments with a carbon-rich surface. The presence of the carbon-rich layer on the surface of the fibers makes them non-wetting to most glasses; hence the fibers are held in the matrix only by frictional forces acting at the interface. The mechanical gripping responsible for the force can be changed by manipulating the glass matrix/fiber thermal expansion coeffi-cient mismatch. Frictional stresses (tau) and friction coefficients (mu) obtained for SiC monofilaments in a soda-lime-silica glass matrix were compared with previously obtained data on a borosilicate glass matrix (tau = 2-3 MPa, mu = 0.72 + or - 0.36). For the sodalime-silica system, tau's of 4-20 MPa and mu of 0.10 + or - 0.03 were obtained. Tau in the soda-lime-silica system is higher due to the larger difference in thermal expansion mismatch between the fiber and matrix. The differences in mu may be due to lubrication effects caused by water at the fiber-matrix interface.

101.126 PB91-203059 Not available NTIS National Inst. of Standards and Technology (IMSE), Boulder, CO. Fracture and Deformation Div.

Monitoring of Anisotropic Material Elastic Properties Using Ultrasonic Receiving Rays.

D. W. Fitting, and A. V. Clark. 1989, 8p Sponsored by National Research Council of Canada, Ottawa (Ontario).

Pub. in Proceedings of International Symposium on Nondestructive Characterization of Materials (3rd), Saarbruchen, FRG, October 3-6, 1988, p91-98 1989.

Keywords: \*Anisotropy, \*Elastic properties, \*Ultrasonic tests, \*Piezoelectric gages, \*Materials tests, On-line measurement systems, Monitors, Measurement, Arrays, Graphite-epoxy composites, Phase velocity, Nondestructive tests, Receivers, Reprints.

A robust technique has been developed for determining the elastic constants of an antistropic material and for on-line monitoring of changes in the elastic proper-ties. Use of an array of small piezoelectric elements as the receiver permits gathering information on the angle-of-arrival of the ultrasonic beam as well as the arrival time. On-line monitoring of changes in the elastic properties of a material is carried out by directing an ultrasound beam from a stationary transmitting transducer into the sample in a specified direction. Alterations in the stiffness constants of the material (as a result of such things as moisture absorption) will cause the direction of the energy flux to deviate. These deviations are readily monitored with the array of receivers. The arrays fabricated for monitoring elastic properties and the electronics required to process their signals are described herein. Use of the arrays for measuring the quasilongitudinal and quasitransverse wave fields in an anisotropic material (graphite-epoxy composite) is described and the importance of the measurement in correctly determining group and phase velocities is discussed.

## Composite Materials

101,127 PB91-203687 Not available NTIS National Bureau of Standards (IMSE), Gaithersburg,

MD. Ceramics Div.
Role of Glassy Interfaces In High Temperature
Crack Growth in SiC Fiber Reinforced Alumina. Final rept.

S. V. Nair, K. Jakus, and C. Ostertag. 1988, 6p Pub. in Proceedings of Annual Conference on Composites and Advanced Ceramic Materials (12th), p681-686 1988.

Keywords: \*Composite materials, \*Ceramic matrix composites, \*Ceramic fibers, \*Fracture mechanics, Aluminum oxide, Silicon carbides, Crack arrest, High temperature tests, Fiber composites, Interfacial tension, Time dependence, Bridging, Temperature de-pendence, Loads(Forces), Borosilicate glass, Coatings(Materials), Crack propagation, Reprints, Fiber pull-out.

Glassy alumina reinforced with continuous SiC fibers and pure alumina reinforced with SiC fibers with and without a coating of a borosilicate glass were studied in this investigation. The experimental component involved conducting constant displacement rate and constant load tests at approximately 1000 C. These tests were interrupted at various times to examine crack morphology changes with temperature and time dependent effects on fiber bridging of cracks. A signifi-cant result was that cracks were found to open in a time dependent fashion by fiber pull out prior to eventual failure. It is shown that such a time dependent interfacial slip can be modeled based on viscous slip in a glassy layer at the fiber/matrix interface.

Not available NTIS PB91-237123 National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Ceramics Div. Differential Sintering.

C. Ostertag. 1991, 7p Pub. in Science of Sintering, p453-459 1991.

Keywords: \*Ceramic matrix composites, \*Fiber composites, \*Sintered materials, Stress relaxation, Stress tests, Crack initiation, Fracture mechanics, Ceramic coatings, Aluminum oxide, Reprints.

The paper discusses an extreme example of differential sintering, namely sintering of fiber-reinforced com-posites. The stress that develops during sintering of composites initiate during the heating cycle, where the matrix has a low density and, hence, a low strength. Crack formation occurs mainly during the stage of sintering. Stress relaxation methods by coating the fibers with coarse-grained alumina particles is being discussed.

101,129 PB91-237321 Not available NTIS National Inst. of Standards and Technology (IMSE), Gaithersburg, MD. Fracture and Deformation Div. Change in Magnetic State of Fe + Silica Gel Nano-composites Due to Low Temperature Treatment in Ammonia. Final rept.

R. D. Shull, J. J. Ritter, and L. J. Swartzendruber. 1991, 3p

Pub. in Jnl. of Applied Physics 69, n8 p5144-5146, 15 Apr 91.

Keywords: \*Magnetic materials, \*Iron compounds, \*Silica gel, \*Composite materials, \*Nanostructures, Ferromagnetic materials, Polymerization, Ambient temperature, Aqueous solutions, Superparamagnetism, Mossbauer effect, Hydrogen, Ammonia, Annealing, Spin glass, Reprints.

Homogeneous gelled composites of iron and silica containing 11-40 wt. % Fe were prepared by room temperature polymerization of aqueous solutions of ferric nitrate, tetraethoxysilane, and ethanol (with an hydrogen fluoride catalyst). The effect on the magnetic state of these nanocomposites following a low temperature (T < 400 C) treatment in 1 atm of ammonia (after a prior anneal in 1 atm of hydrogen) is presented, along with the dependence on the H2 pretreatment. In all cases the room temperature Mossbauer spectra for the material in the NH3-treated and H2-pretreated conditions were similar. However, when treated in H2 at 770 C (2 h) the Mossbauer spectra also contained a significant component having a large isomer shift (1.3 mm/s) and quadrupole splitting (3.2 mm/s). The material was also slightly ferromagnetic at all temperatures below 300 K. For materials pretreated in hydrogen below 400 C, a threefold enhancement in the magnetic susceptibility was measured following treatment in ammonia. In addition, both the field and temperature dependence of the susceptibility indicated the presence of spin-glass behavior at 10 K for NH3-treated samples containing up to 40% Fe. At room temperature, these latter ammonia-treated nanocomposites were either superparamagnetic (Fe contents, C(sub Fe) up to 25%) or ferromagnetic (C(sub Fe) <25%).

PB92-117258 Not available NTIS National Inst. of Standards and Technology (CSTL), Boulder, CO. Chemical Engineering Div.

Thermal Conductivity of Alumina Fiber/Epoxy and Alumina Fiber/PEEK from 4.2 to 310 K. Final rept.

D. L. Rule, and L. L. Sparks. 1990, 15p See also PB89-218358.

Pub. in Proceedings of International Thermal Conductivity Conference (21st), Lexington, KY., October 15-18, 1989, p671-685 1990.

Keywords: \*Thermal conductivity, \*Peek, \*Epoxy matrix composites, \*Polymer matrix composites, \*Resin matrix composites, \*Fiber composites, Temperature dependence, Aluminum oxides, Ceramic fibers, Thermal cycling tests, Orientation, Measurement, Reprints.

The thermal conductivities of poly-ether-ketone (PEEK), of alumina fiber in a matrix of PEEK, and of alumina fiber in a matrix of epoxy were determined along with the effects of fiber orientation and thermal cycling. Thermal conductivity was measured over the temperature range 4.2 to 310 K using a steady-state apparatus. These data are presented and discussed relative to specimen characteristics. After different fiber fractions in the specimens were accounted for, the thermal conductivity of the PEEK composite material is less than that of the epoxy composite material in particular temperature ranges for the heat flow parallel to the fiber direction.

101.131

PB92-117332 Not available NTIS National Inst. of Standards and Technology (MSEL), Magnetic Behavior of Nanocomposites Prepared

in a Vitreous Alumina Gel. Final rept.

Final rept.

R. D. Shull, J. J. Ritter, A. J. Shapiro, L. J.

Swartzendruber, and L. H. Bennett. 1991, 6p

Pub. in Materials Research Society Stmposia Proceedings, v206 p455-460 1991.

Keywords: \*Ceramic matrix composites, \*Gels, \*Aluminum oxides, \*Polymerization, \*Iron compounds, Magnetic materials, Iron nitrates, Aqueous solutions, Vitreous state, Alcoholates, Ferromagnetism, Nitric acid, Electron microscopy, X-ray diffraction, Mossbauer effect, Embedding, Magnetic permeability, Temperature dependence, Hydrogen, Production (Chemiston Programme Resident Note) perature dependence, Hydrogen, Reduction(Chemistry), Paramagnetism, Reprints, Nanocomposites.

Homogeneous gelled composites of iron and vitreous alumina containing 10-40% Fe have been prepared by room temperature polymerization of aqueous aluminum alkoxide solutions containing ferric nitrate and nitric acid at low pH. Scanning electron microscopy, xray diffraction, and Mossbauer spectroscopy demonstrated that this bulk material is comprised of nano-meter-sized regions of iron compounds embedded in a vitreous alumina gel matrix. Magnetization data showed that in the as-cured condition these nanocomposites areparamagnetic at room temperature and become either superparamagnetic or ferromagnetic on cooling to 10 K. The magnetic susceptibility increased with the Fe content and with decreasing temperature.

Analysis of the temperature dependence of the magnetic susceptibility indicated the magnetic moment per Fe atom was 1.87 for the 10% Fe nanocomposite and that it increased linearly with composition to 1.96 for the 40% Fe material. Mossbauer effect data showed that subsequent treatment of these materials in a gaseous environment of hydrogen at elevated temperatures (T<400 C) changed the form of the iron in the magnetic regions. These results are compared to that observed for similar nanocomposites prepared using a silica gel matrix.

#### Corrosion & Corrosion Inhibition

101.132

PB91-134700 Not available NTIS National Bureau of Standards (IMSE), Gaithersburg,

MD. Metallurgy Div.
Corrosion, Repassivation and Corrosion Fatigue Behavior of the Surgical Implant Alloy, Co-Cr-Mo. Final rept.

P. Sung, and A. C. Fraker. 1987, 10p
Pub. in Proceedings of Conference on Environmental
Degradation of Engineering Materials III, University
Park, PA., April 13-15, 1987, p471-480.

Keywords: \*Cobalt alloys, \*Chromium alloys, \*Molybdenum alloys, \*Corrosion alloys, Surgical transplanta-tion, Implantation, Orthopedics, Passivity, Bones, Joints(Anatomy), Reaction kinetics, Surface chemistry, Protective coatings, Fatigue life, Reprints.

The cobolt-chromium-molybdenum (Co-Cr-Mo) alloy is used widely as an orthopedic surgical implant material. In-vivo degradation of the alloy due to corrosion or corrosion fatigue can lead to metal ion release into the body or fracture of the device. The continual destruction of the protective film can promote crack formation and thereby cause fracture of the implant. Scully, and Ambrose and Kruger were among the earliest workers to emphasize the importance of passive film and re-passivation results in the metal ions adjacent to the ruptured films being dissolved before another protective film can be formed. However, if the repassivation rate is much faster than the rate of film rupture, metal ions may not be dissolved, and corrosion may not occur. By monitoring the current transient after a bare metal surface is formed by abrading, while maintaining a constant potential with a potentiostat, the repassivation kinetics can be measured.

101.133

PB91-149047 Not available NTIS National Bureau of Standards (IMSE), Gaithersburg, MD. Metallurgy Div.

Cleavage Step Formation and Resistance to Transgranular Stress Corrosion Cracking. Final rept.

E. N. Pugh, and M. J. Kaufman. 1986, 11p Pub. in Proceedings of Materials Technology Con-gress, Adelaide, Australia, May 19-21, 1986, v2 p1-11.

Keywords: \*Stress corrosion, \*Metals, \*Fracture mechanics, \*Transgranular corrosion, Crack propagation, Clevage, Embrittlement, Shear strength, Precipitation hardening, Reprints.

A new approach to improving the resistance of alloys to transgranular SCC is described. It is based on the view that this important service failure occurs by discontinuous cleavage and that resistance to this form of cracking can be achieved by impeding the formation of steps between parallel but displaced cleavage facets. It is suggested that the steps in the case of susceptible alloys are produced by plastic shearing on slip planes, and that this low energy process can be restricted either by ensuring that ready cross-slip can occur (by avoiding low stacking fault energy and short range order) or by increasing the shear strength by precipita-tion hardening. This approach does not affect the in-trinsic susceptibility of the material but is designed to impart resistance by inhibiting crack propagation. The approach also provides new insight into the mechanism of the embrittlement process.

101,134

PB91-150078 Not available NTIS National Inst. of Standards and Technology (IMSE), Gaithersburg, MD. Metallurgy Div. Concepts of Underground Corrosion.

Final rept.

E. Escalante. 1989, 14p
Pub. in Effects of Soil Characteristics on Corrosion. ASTM STP 1013, p81-94 1989.

Keywords: \*Metals, \*Electrochemical corrosion, \*Soil properties, \*Steels, Soil microbiology, Electrical resistivity, Aeration, Oxygenation, Reprints.

Corrosion in soil is a complex phenomenon, but there are some basic concepts that are useful in understanding the process. Underground corrosion is electrochemical in character, and this fact is used to describe the corrosion process in terms of an ordinary dry cell. The differences between corrosion in disturbed and undisturbed soil are discussed, and data

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## Corrosion & Corrosion Inhibition

are presented to emphasize these differences. The results reveal that soil composition is less important than soil resistivity, but both are subordinate in importance to oxygen availability. Thus, corrosion is negligible in undisturbed soils where oxygen concentration is low.

101,135 PB91-158667 Not available NTIS National Bureau of Standards (IMSE), Gaithersburg, MD. Metallurgy Div.
Corrosion Testing in Soil. Final rept.

E. Escalante. 1987, 4p

Pub. in Metals Handbook, v13 p208-211 1987.

Keywords: \*Corrosion tests, \*Soils, \*Metals, Measurement, Underground corrosion, Sampling, Oxygen, Design criteria, Reprints.

An approach to evaluating the durability of a metal in soil will be described. Specimen design, preparation, burial, and retrieval techniques will be discussed. The type of information sought during soil-induced corrosion evaluation controls the design configuration and he nature of the corrosion measurements. Consideration of these factors during the planning stage will help the corrosio engineer obtain a maximum amount of information with a minimum number of future prob-lems in the program. The corrosion of metals underground can be divided into two broad categories: corrosion in undisturbed soils and corrosion in disturbed soils. Corrosion in undisturbed soil is always low, regardless of soil conditions, and is limited only by the availability of the oxygen necessary for the cathodic reaction. Steel piles driven into soil fall under this category and therefore undergo limited corrosive attack.

101,136 PB91-174714 Not available NTIS National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Metallurgy Div.

Measuring the Corrosion of Metals in Soil. Final rept.

Pub. in Corrosion Testing and Evaluation: Silver Anniversary Volume, ASTM STP 1000, p112-125 1990.

Keywords: \*Soils, \*Underground corrosion, \*Copper, Corrosion tests, Measurement, Polarization, Galvanic corrosion, Alternating current, Pile structures, Re-

Polarization resistance and galvanic current measurements, used for underground corrosion studies, are described, and problems encountered in making these measurements in the field, along with solutions, are discussed. Polarization measurements, supported by physical measurements, have shown that induced al-ternating current increases the corrosion rate of copper concentric neutrals compared to copper neutrals without ac. These measurements also revealed that driven piles undergo less corrosion attack than similar piles in backfilled trenches. Galvanic current measurements provide valuable information on the behavior of galvanically coupled materials and can be used to compare the corrosivity of soil environments.

101,137 PB91-175182 Not available NTIS National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Metallurgy Div.

Stress Corrosion Cracking of Al-Li Alloys: The Role of Grain Boundary Precipitates.

Final rept.

R. E. Ricker, J. L. Fink, and A. K. Vasudevan. 1991,

Pub. in Metallurgical Transactions A 22A, p264-267

Keywords: \*Aluminum alloys, \*Lithium alloys, \*Stress corrosion cracking, Grain boundaries, Precipitates, Precipitation hardening, Microstructure, Heat treatment, Copper alloys, Binary alloys, Ternary alloys, Yield strength, Fracture mechanics, Reprints.

The stress corrosion cracking (SCC) behavior of pre-cipitation hardened alloys may depend on a large number of microstructural parameters that vary during fabrication and heat treatment such as grain size, grain boundary (gb) solute segregation, precipitate size, pre-cipit free zone, and matrix slip character. Since all of these factors vary simultaneously during normal heat treatments, it is difficult to assess independently the contribution of each microstructural factor to the SCC behavior of the alloy. In particular, a series of experiments were designed which would allow the evaluation

of the role of gb precipitates in the SCC behavior of Al-Li and Al-Li-Cu alloys independent of the other factors (such as matrix precipitate microstructure) that normally vary during aging treatments. For these experiments, the matrix precipitates of a binary Al-Li alloy were held constant, keeping the yield strength constant, while the gb precipitate size and volume percent were systematically varied. In contrast, to keep the yield strength of the ternary Al-Li-Cu alloy constant at the same level as the binary alloy, the matrix precipi-tate size and distribution were varied with the gb pre-

101,138

PB91-187690 PC A03/MF A01 National Inst. of Standards and Technology (BFRL), Gaithersburg, MD.

Chloride Ion Diffusion in Low Water-to-Solid Chloride Ion Diffusion in Low Water-to-Solid Cement Pastes.
J. R. Clifton, L. I. Knab, E. J. Garboczi, and L. X. Xiong. Apr 91, 31p NISTIR-4549
Prepared in cooperation with Shanghai Research Inst.

(China). Sponsored by Nuclear Regulatory Commission, Washington, DC.

Keywords: \*Corrosion tests, \*Reinforced concrete, \*Composite materials, \*Reinforcing steels, \*Chlorine ions, Diffusion, Portland cements, Moisture content, Mathematical models, Service life, Performance prediction, Radioactive waste management, Low-level radioactive wastes.

Diffusion coefficients of 0.3 water to solids ratio (w/s) hydrated portland cement paste specimens were measured using a conventional diffusion cell. Specimens were made from both ASTM Type I and Type II portland cements and blends containing mineral admixtures (fly ash, granulated blastfurnace slag, or silica fume). The average diffusion coefficient for the portland cement paste specimens was 14x10(sup -13)sq m/s. The effects of the depth of concrete cover over reinforcing steel and of the chloride ion diffusion coeffi-cient on the service life of reinforced concrete exposed to chloride ions were predicted based on a diffusion model. Based on the model, the effect of the cover was shown to be proportional to the square of the cover depth. A 10-fold decrease in the diffusion coefficient of concrete was predicted to result in a 10fold increase in the predicted service life.

101.139

PB91-203588 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Building Materials Div.

Detection and Quantitative Characterization of Blistering and Corrosion of Coatings on Steel Using Infrared Thermography.

Final rept. M. E. McKnight, and J. W. Martin. 1989, 6p Contract NCEL-86WR60188 Sponsored by Naval Civil Engineering Lab., Port Hue-

Pub. in Jnl. of Coatings Technology 61, n775 p57-62 Aug 89.

Keywords: \*Protective coatings, \*Structural steels, \*Barrier materials, \*Corrosion prevention, Corrosion products, Characterization, Weathering, Quantitative analysis, Thermography, Blisters, Infrared thermal detectors, Process variables, Air flow, Organic compounds, Thickness, Image analysis, Time dependence, Panels, Construction materials, Interfaces, Reprints prints.

Results of studies to assess the effect of several key experimental variables on the detection of blisters and corrosion spots at the interface of organic coatings and steel using infrared thermography are presented. Coating defects, such as blisters and corrosion spots, are detected as a result of differences in the thermal properties of degraded and non-degraded areas of a coated panel when a temperature gradient is induced through the thickness of the coated panel. The resulting thermographic image is then analyzed using com-puter image processing to determine size, location and extent of degradation. Therefore, the method provides a quantitative, nondestructive procedure for determin-ing the extent of deterioration on coated metal panels. The results of the studies show that experimental variables such as the method of heating test panels, the panel temperature, the flow rate of air, the time between initiation of heating and acquisition of the thermographic image and the thickness of the organic coatings can affect the results.

#### **Elastomers**

101,140

PB91-132167 PC A03/MF A01 National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Center for Fire Research.

Reduction of Hydrogen Cyanide Concentrations and Acute Inhalation Toxicity from Flexible Polyurethane Foam Combustion Products by the Addition of Copper Compounds. Part 3. The Effect of Copper Additives on the Flammability Characteristics of Flexible Polyurethane Foam.

B. C. Levin, E. Braun, J. R. Shields, and D. Lowe. Oct 90, 39p NISTIR-4441

Sponsored by International Copper Research Association, Inc., New York, and Society of the Plastics Industry, Inc., New York.

Keywords: \*Hydrogen cyanide, \*Combustion products, \*Copper compounds, \*Foam rubber, \*Polyure-thane resins, Exhaust gases, Flammability testing, Toxicity, Thermal degradation, Respiration, Statistical analysis, Heat measurement, Ignition, Oxidation.

The report addresses the issue of whether the addition of a copper compound to a flexible polyurethane foam would affect the flammability characteristics of the foam. The following properties were examined: (1) ignitability in three systems (the NBS Toxicity Test Method, the Cone Calorimeter, and Lateral Ignition and Flame Spread Test (LIFT)), (2) heat release rate under small-scale (Cone Calorimeter) and mediumscale (furniture calorimeter), (3) smoke obscuration (Cone Calorimeter), and (4) rate of flame spread (LIFT). In all cases, no differences in flammability characteristics between the treated and untreated foam were observed.

101,141

PB91-195081 Not available NTIS National Bureau of Standards (IMSE), Gaithersburg, MD. Polymers Div.

Mechanical and Swelling Behavior of Crosslinked Natural Rubber: Consequences of the Flory-Rehner Hypothesis.

Final rept.

G. B. McKenna, K. M. Flynn, and Y. Chen. 1988, 4p Pub. in Polymer Communications 29, n9 p272-275 Sep

Keywords: \*Natural rubber, \*Swelling, \*Crosslinking, Networks, Benzene, Methyl ethyl ketone, Ethyl acetate, Acetone, Density(Mass/Volume), Elastic properties, Heat of mixing, Reprints, \*Flory-Rehner hypothesis, \*Flory-Huggins parameter, Dicumyl peroxide.

The Frenkel-Flory-Rehner (FFR) hypothesis that the elastic free energy of a swollen network is balanced by the free energy of mixing has been examined using experiments on dicumyl peroxide crosslinked natural rubber. Swelling was performed in good solvent (benzene) and poor solvent (Methyl ethyl ketone, Ethyl acetate, acetone) conditions crosslink density varied from 2.3 x 10(sup -5) to 3.26 x 10(sup -4) moles/cu m. Validity of the FFR hypothesis demands that the Flory-Huggins interaction parameter, chi, in the expression for the free energy of mixing be dependent upon the crosslink density, upsilon. Then it is found that there is an apparently universal relationship between the volume fraction of rubber, v2, and the effective interaction parameter chi (effective), viz, v2 = v2 (chi (effective)) = upsilon2 (chi, upsilon). The value of chi (effective) tive) depends upon crosslink density as (chi (effective) - chi(0)) = (a)upsilon where for the natural rubber and solvents studied appears to be independent of solvent.

#### **Fibers & Textiles**

101,142

PC A02/MF A01 AD-A236 708/4 National Inst. of Standards and Technology (IMSE), Gaithersburg, MD. Ceramics Div.

## Fibers & Textiles

Effects of Multiple Filament Geometry in the Hot Filament Deposition of Diamond Films.

Interim rept. E. N. Farabaugh, A. Feldman, and L. H. Robins. 12 Apr 91, 9p

Contract N00014-90-F-0011

Keywords: Chambers, Deposition, \*Diamonds, Feeding, \*Filaments, Films, Flow rate, Gas flow, Gases, Geometry, Growth(General), High rate, Hot wire, Morphology, Parameters, Pressure, Rates, Surface properties, Volume, Methane, Pyrolysis.

Scaleup of hot filament chemical vapor deposition of diamond films requires knowledge of how filament geometry affects the deposition process. The effect of multiple filament geometry on the growth rate and surface morphology of diamond films is presented. Three factors were varied: the number of helical turns in a filament - 5, 10 or 15; the number of filaments present --1 or 2; and the CH4 fraction in the CH4-H2 feed gas mixture -- 0.25%, 0.5%, 0.75% or 1.0%. Other depositions parameters were 750 C substrate temperature, 52 standard cm/m total feed gas flow rate, and 5300 Pa deposition pressure. The deposition chamber volume was 1.9 liters. Increasing the CH4 concentration in the feed gas results in higher growth rates. However, increasing the number of filament turns in dual filament systems resulted in lower than expected growth rates for dual 10 and 15 turn filaments.

Not available NTIS PB91-149948 National Inst. of Standards and Technology (NML), Boulder, CO. Chemical Engineering Science Div. **Round Robin on Apparent Thermal Conductivity of** Several Loose-Fill Insulations. Final rept.

R. D. Adams, and J. G. Hust. 1990, 27p Sponsored by Oak Ridge National Lab., TN.
Pub. in Insulation Materials, Testing, and Applications,
ASTM STP 1030, p263-289 1990.

Keywords: \*Thermal insulation, \*Thermal conductivity, \*Interlaboratory comparisons, Cellulose, Rock wool, Glass fibers, Fabrics, Measurement, Precision, Bias, Fillers, Reprints.

The primary means of establishing the thermal per-formance of loose-fill insulation is ASTM Standard Practice C 687. To provide information for the development of a statement of precision and bias for the Standard Practice, a round robin was carried out by eleven laboratories measuring apparent thermal con-ductivity of four common loose-fill insulation products (cellulose, rock/slag wool, and bonded and unbonded glass fiber) and a glass fiber blanket. The test results on the glass fiber blanket indicate that the measurement capability of the participants can be characterized by an imprecision of 3.0%, as measured by two standard deviations, and a negligible bias of the mean. The measurements on the loose-fill materials are characterized by an imprecision ranging from 21% for cellulose to 10% for the rock/slag wool. The increase in imprecision for the loose-fill materials is attributed primarily to inadequately defined procedures for preparing and conditioning the specimens.

### Iron & Iron Alloys

101.144 N91-20218/4

(Order as N91-20207/7, PC A05/MF A01) National Bureau of Standards (IMSE), Gaithersburg, MD.

Low Carbon Steel: Metallurgical Structure vs. Mechanical Properties.

R. D. Shull. Jan 90, 4p In NASA, Langley Research Center, National Educators' Workshop: Update 1988. Standard Experiments in Engineering Materials Science and Technology p

Keywords: Experimentation, \*Low carbon steels, \*Mechanical properties, \*Metallurgy, Heat treatment, Low cost, Phase diagrams, Pins, Procedures, Students, Temperature effects, \*Thermomechanical treatment.

The objective is to provide a low cost, simple experiment for either demonstration purposes or as a labora-tory experiment that will teach the student the importance of the thermal-mechanical history of a metallic alloy in determining that material's mechanical behavior. Hairpins are subjected to various treatments. The experimental equipment and procedures are discussed.

PB91-134627 Not available NTIS National Inst. of Standards and Technology (IMSE), Boulder, CO. Fracture and Deformation Div.

Cryogenic Material Properties of Stainless Steel

Tube-to-Flange Welds. Final rept.

T. A. Siewert, C. N. McCowan, and D. P. Vigliotti. 1990, 9p

Pub. in Cryogenics 30, p356-364 Apr 90.

Keywords: \*Chromium nickel alloys, \*Weldments, \*Manganese alloys, \*Cryogenics, Pipes(Tubes), Mechanical properties, Superconductors, Flanges, Tension tests, Tensile strength, Notch strength, Fatigue life, Failure, Thermal cycling tests, Loads(Forces), Reprints, \*Stainless steel-304L, \*Stainless steel-316L, Superconducting super collider.

The mechanical properties of stainless steel tube-toflange welds for a cryogenic piping application were measured. A planar specimen was developed to duplicate the constraint, loading and heat-sink properties of the circular joint, while reducing preparation time and cost. Specimens were evaluated containing welds between the tube material (21Cr-6Ni-9Mn) and the three stainless steels being considered for the flange materials: type 304L, type 316L and 21Cr-6Ni-9Mn. The mechanical property tests consisted of three phases: simple tensile testing to failure, tensile testing of notched specimens (where the notch simulated fabrication flaws) and fatigue testing of notched specimens for the 4 x 10(sup 4) cycle design life of the structure. The type 316L stainless steel flange produced welds with the best combination of strength and ductility at 295 and 4K in all three phases of testing.

101,146 PB91-147686 Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Building Materials Div.

Roughness Measures of Blasted Steel Surfaces Remotely Imaged with a Thermographic Camera. Final rept.

J. W. Martin, and D. P. Bentz. 1987, 18p Pub. in Proceedings of Symposium on Corrosion Protection by Organic Coatings, v87-2 p179-196 1987.

Keywords: \*Surface roughness, \*Steels, \*Panels, \*Thermography, \*Abrasive blasting, Abrasion, Surface properties, Roughness, Profilometers, Finishes, Blasting, Reprints.

A standard series of blasted steel panels were imaged with a thermographic camera and characterized with respect to surface roughness using fractal and depth mapping techniques. It was shown that the fractal dimensions of these blasted steel panels correlate very well with their perceived roughness and that a computer rendering of a fractal surface looks like a blasted surface. At present, depth mapping on blasted steel substrates is too complicated to perform; instead, a series of precision drilled and milled holes were used. For milled holes, a good relationship exists between thermographically and physically measured diameter and depth measurements. For drilled holes, a good relationship exists for diameter, but not depth, since the emission effects of hole depth and drill angle have not been separated out.

Not available NTIS PB91-148106 National Bureau of Standards (IMSE), Gaithersburg, MD. Metallurgy Div.
Study of the Galling of Two Steels Using Two Test

Methods.

Final rept. P. A. Swanson, L. K. Ives, E. P. Whitenton, and M. B. Peterson. 1988, 17p Pub. in Wear 122, n2 p207-223, 1 Mar 88.

Keywords: \*Tribology, \*Steels, \*Galling, Wear tests, Measurement, Carburizing, Quenching(Cooling), Comparison, Methodology, Reprints, \*Steel-AISI-1541, parison, Steel-AISI-8620.

The galling behavior of two heat treated steels, AISI 1541 and 8620, was investigated. Two laboratory tests were used. The first utilized a sphere-on-flat contact geometry and the second a flat-on-flat geometry. The galling damage that was generated was measured by

using a stylus profilometer to collect a series of parallel profiles through the damage zone. The maximum peak-to-valley distance for each profile was calculated and the average of this parameter was then used to quantify the amount of galling that was produced. The measurement technique enabled the authors to not only assess the galling behavior of the test materials but it also allowed the authors to determine the variability inherent in each test method. Significantly less damage was obtained for carburized 8620 on quenched' 1541 steel than was observed when the quenched 1541 steel was tested under self-mated conditions. The greatest amount of damage was generated when hot-rolled 1541 steel was run against itself. Possible reasons for these results will be re-

101,148

PB91-158980 Not available NTIS National Inst. of Standards and Technology (MSEL), Boulder, CO. Fracture and Deformation Div. Fracture Toughness of 316L Stainless Steel Welds with Varying Inclusion Contents at 4 K.

Final rept.

C. N. McCowan, and T. A. Siewert. 1990, 8p Sponsored by Department of Energy, Washington, DC Pub. in Advances in Cryogenic Engineering (Materials), v36 p1331-1338 1990.

Keywords: \*Fracture strength, \*Stainless Steel-316L, \*Weld defects, \*Inclusions, Hardness, Welding, Stainless\_steels, Loads(Forces), Voids, Cracks, \*Cryogenics, Reprints.

The 4K fracture toughness of a type 316L stainless steel weld composition increased significanlty when the inclusion contents of the GMA welds were decreased. For the three welds tested (Ni-13 wt. 4K yields strngth approx. 740 MPa), the fracture toughness increased 35% as the inclusion contents were decreased by 65%. Expressing the effect of inclusions on the toughness in terms of the inclusion spacing (inverse square root of the inclusion density), the fracture toughness of the 316L welds increased 18 MPa.m(exp 1/2) per micron increase in the average inclusion spacing. Fractographic studies were conducted to characterize differences in the initiation of fracture as a function of the inclusion content. Fracture specimens that were examined after loading into the blunting range had stable crack growth lengths of 0.1 to 0.25 mm. Crack growth occurs as voids which formed at inclusions link by microcracking, rather than coales-

101.149

PB91-167171 PC A03/MF A01 National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Metallurgy Div.

**Examination of the Excessive Retained Austenite** on the Surface of a Section of 17-7 Precipitation Hardening Stainless Steel.

G. E. Hicho, W. J. Boettinger, L. Swartzendruber, and T. R. Shives. Jan 91, 32p NISTIR-4502

Keywords: \*Austenite, \*Stainless steels, \*Chromium-nickel steels, Surface properties, Precipitation harden-ing, Heat treatment, Microstructure, Aluminum addi-

A 'mishap' section, and other selected sections made from 17-7 precipitation hardening stainless steel were metallurgically examined, and it was concluded that the unusually large amount of retained austenite, greater than 7%, measured on the surface appears to have been produced during both the solution annealing and austenite conditioning steps of the heat treating process, but was revealed only after the austenite conditioning step. It is suspected that the excessive retained austenite occurred during the heat treating process where these sections may have been exposed to a furnace atmosphere that contained too much carbon or nitrogen. The exposure could have led to an increase in the amount of retained austenite both on the surface and internally

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PB91-167346 PC A03/MF A01 National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Metallurgy Div.

# Iron & Iron Alloys

Crack Arrest Fracture Toughness Measurements of Normalized and Inclusion Shape Controlled AAR TC128 Grade B Steel, and Micro-Alloyed, Control-Rolled, and Inclusion Shape Controlled A 8XX Grade B Steel

G. E. Hicho, Feb 91, 18p NISTIR-4501, REPT-21

Keywords: \*Fracture mechanics, \*Carbon steels, \*Railroad cars, Tank cars, Fracture strength, Crack arrest, Measurement, Inclusions, Process variables, Process control.

The crack arrest fracture toughness was determined for normalized AAR TC 128 grade B steel and control rolled A 8XX grade B steel. Both steels were made using inclusion shape control practice. The crack arrest fracture toughness of the AAR TC 128 steel was slightly better than that for the A 8XX steel.

101,151 PB91-175372 Not available NTIS National Inst. of Standards and Technology (IMSE), Boulder, CO. Fracture and Deformation Div. Effect of Nitrogen and Carbon on FCC-HCP Stability in Austenitic Steels. Final rept.

R. P. Reed, and M. W. Austin. 1989, 4p Pub. in Scripta Metallurgica 23, n8 p1359-1362 1989.

Keywords: \*Austenitic steels, \*Nitrogen additions, Austenite, Ferrite, Martensitic transformation, FCC lattices, HCP lattices, \*Carbon additiions, Reprints.

High-nitrogen austenitic steels have recently been developed for low-temperature use. For a long time it has been recognized that both nitrogen and carbon increase austenite stability with respect to formation of delta ferrite at high temperatures and body-centered cubic (bcc) martensite at low temperatures. Yet, the effects of nitrogen and carbon on austenite (fcc) stability relative to hexagonal close-packed (hcp) martensite and the stacking-fault energy have not been adequately clarified.

101,152 PB91-175448 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Surface Science Div. Mechanical Sputtering of Structural Stainless Steels.

Final rept.

T. Nenadovic, N. Popovic, and J. Fine. 1989, 8p Pub. in Jnl. of Materials Science 24, p3699-3706 1989.

Keywords: \*Sputtering, \*Austenitic stainless steels, \*Erosion, Structural steels, Gas turbine blades, Pressure vessels, Deterioration, Wear, Surfaces, Pitting,

In the paper the results of an investigation of the beam modification (erosion) of stainless steel are presented. The possible similarity of the martensitic stainless steel degradation for turbine engine blades and austenitic stainless steel used as a wall of the vacuum vessel for fusion reactor application has been pointed out. Changes appearing during the interaction have been investigated on the rotating turbine blade material. Simultaneously morphological changes of the 'target' and the change of shape of bombarding species have been analyzed.

101,153 PB91-184747 PC A03/MF A01 National Inst. of Standards and Technology (MSEL), Boulder, CO. Materials Reliability Div. Microstructure, Composition, and Hardness of Rockwell C Hardness Blocks. T. A. Siewert, and A. Tomer. Jan 91, 26p NISTIR-

3960

Keywords: \*Rockwell hardness, \*Standards, \*Steels, Compositions, Microstructure, Hardness, Purity.

The microstructure, composition, and hardness of hardness blocks (Rockwell C scale) that are commonly available in the country were examined. Blocks near HRC levels of 25, 45, and 65 were obtained from each of six sources to represent the HRC measurement range. It was found that the steels used in the blocks had surprisingly high levels of impurity elements, which are one source of scatter in the hardness values. Other than the concern for the steel purity, it is con-cluded that most of these hardness block producers possess the technology necessary to manufacture a reference hardness block, or series of blocks, if it is found desirable for NIST to distribute a national hardness standard.

101,154 PB91-184838 PC A03/MF A01 National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Center for Fire Research.

Prediction of Elevated Temperature Deformation

of Structural Steel under Anisothermal Conditions. B. A. Fields, and R. J. Fields. Jan 91, 46p NISTIR-4497

Sponsored by American Iron and Steel Inst., Washing-

Keywords: \*Structural steels, Performance prediction, High temperature tests, Deformation, Strain tests, Creep properties, Computer programs, Heating, Elas-tic properties, Equations, Tables(Data), Strain harden-ing, Steel-ASTM-A36, Anisothermal.

Using a previously formulated equation which calculates the elastic, plastic and creep strains during loading at a constant elevated temperature, a method and a computer program have been developed that will predict the strain due to creep during anisothermal tests at constant load. Comparisons were made with results from anisothermal tests for AS A149, an Australian steel close to the specification for ASTM A36. Agreement is excellent for several linear heating rates and one nonlinear heating rate.

101,155 PB91-187856 PC A03/MF A01 National Inst. of Standards and Technology (MSEL), Boulder, CO. Materials Reliability Div. Continuous-Cooling Transformation Characteris-

tics and High-Temperature Flow Behavior of a Mi-croalloyed SAE 1141 Steel. Y. W. Cheng, and A. Tomer. Feb 91, 39p NISTIR-

3964

Prepared in cooperation with Israel Atomic Energy Commission, Beersheba Nuclear Research Center-

Keywords: \*Low carbon steels, \*Heat resistant alloys, \*Thermomechanical treatment, Temperature dependence, Phase transformations, Stress tests, Deformation, Fluid flow, Viscosity, Flow stress, Austenite, Ferrite, Pearlite, Microstructure, Crystallization, Automobiles, \*Steel-SAE-1141, \*Microalloyed steels, Continuous cooling

The report presents the results of a thermomechanical processing (TMP) study on a microalloyed SAE 1141 forging steel. The primary objective of the study is to investigate the effects of deformation temperature on the phase-transformation kinetics and to determine the high-temperature flow characteristics of the steel. One-hit compression tests at a constant true strain rate of 10/s were performed with a TMP simulator. Tests were performed at 900, 1000, and 1100 C. The results show that flow stress increased with decreasing temperature. In the strain range 0.35 to 0.6, the effect of temperature on the flow stress can be described by the equation, sigma (MPa) = 2.93 exp (4944/T (K)). Continuous-cooling transformation (CCT) diagrams determined following deformation at 1000 and 1100 C were similar. However, deformation at 900 C shifted the ferrite-plus-pearlite nose to a shorter time and produced a much finer ferrite-plus-pearlite microstructure. This is because the steel does not recrystallize at 900 C after deformation imposed in the study. The usefulness of the CCT diagram and the relationship between deformation and austenite recrystallization are discussed.

PB91-189464 Not available NTIS National Bureau of Standards (IMSE), Gaithersburg, MD. Metallurgy Div.

Effects of Varying Austenitizing Temperature and Cooling Rate on the Ability of HSLA-80 Steel to Achieve a Yield Strength Comparable to HSLA-100.

Final rept.

G. E. Hicho, and R. J. Fields. 1988, 9p Sponsored by David Taylor Research Center, Bethesda. MD.

Pub. in Jnl. of Heat Treating 6, n2 p77-85 1988.

Keywords: \*Austenitic steels, \*Yield strength, \*Heat treatment, Tensile strength, Quenching(Cooling), Temperature dependence, Metal plates, Optimization, Rates(Per time), Reaction kinetics, Thickness, High strength steels, Low alloy steels, Reprints, \*Steel HSLA-80, \*Steel HSLA-100.

Heat treating experiments were conducted on HSLA-80 in order to maximize the yield strength. The paper

concentrates on the optimization of the austenitizing treatment and the cooling rate. The optimum austenitization temperature was found to vary with plate thickness. In all cases, the time-at-temperature was 60 minutes followed by an immersion in water. Double austenitization and other cooling rates did not significantly improve the yield strength. A heat treatment was found for the 19 mm and 32 mm thick plates that improved the yield strength beyond those specified for HSLA-

101,157 PB91-189944 Not available NTIS National Inst. of Standards and Technology (MSEL), Boulder, CO. Fracture and Deformation Div. Influence of Interstitial Content on Fracture Toughness.

Final rept.
P. T. Purtscher, and R. P. Reed. 1989, 5p
Pub. in Proceedings of International Conference on
High Nitrogen Steels, Lille, France, May 18-20, 1988,
p189-193 1989.

Keywords: \*Interstitials, \*Crystal defects, \*Cryogenics, \*Austenitic steels, \*Fracture mechanics, Martensitic transformation, Fracture strength, Tension tests, Ductility, Nitrogen additions, Inclusions, Metallography, Nucleation, Yield strength, Mathematical models, Voids, Stress concentration, Reprints.

The effects of interstitial content on tensile properties, martensitic transformation, and inclusion content are examined in relationship to the measured fracture toughness of austenitic stainless steels at cryogenic temperatures. Metallographic sections show that void nucleation occurs ahead of a crack only after the applied J exceeds a large fraction of the measured toughness, J(sub Ic). A stress intensity factor is calculated for void nucleation from a simple model that considers the yield strength and inclusion spacing.

101.158 PB91-189951 Not available NTIS National Inst. of Standards and Technology (MSEL), Boulder, CO. Fracture and Deformation Div. Metallographic Study of the Crack-Tip Region from Fracture Mechanics Specimens of Austenitic and Ferritic Steels. Final rept.

P. T. Purtscher, R. P. Reed, and D. K. Matlock. 1989,

Sponsored by Department of Energy, Washington, DC. Pub. in Proceedings of MRS International Meeting on Advanced Materials, Tokyo, Japan, May 31-June 4, 1988, p391-396 1989.

Keywords: \*Fracture mechanics, \*Crack opening displacement, \*Austenitic steels, \*Ferritic stainless steels, \*Strain hardening, Fracture strength, Electron microscopy, Etching, Metallography, Microhardness, Publik, Report Ductility, Reprints.

Metallographic sections of blunted and growing cracks in steels with different strain-hardening capacities are observed in the light and scanning electron microscope. The strain distribution around the crack-tip region is inferred from the etching behavior and microhardness readings. The direction of initial growth is approximately straight ahead of the fatigue precrack in the high strain-hardening austenitic steels and at an angle of about 45 degrees in the low strain-hardening ferritic steel. These observations are discussed in terms of different criteria for ductile fracture in fracture mechanics specimens.

PB91-189977 Not available NTIS National Inst. of Standards and Technology (MSEL), Boulder, CO. Fracture and Deformation Div. Discontinuous Yielding during Tensile Tests at Low Temperatures. Final rept.

R. P. Reed, and N. J. Simon. 1990, 10p Sponsored by Department of Energy, Washington, DC. Pub. in Advances in Cryogenic Engineering, v36 p1077-1086 1990.

Keywords: \*Tensile tests, \*Austenitic steels, \*Low temperature tests, Yield strength, Temperature effects, Stresses, Strains, Mechanical properties, Yield point, Tensile properties, Compressive properties, Re-

The effects of temperature and coolant on the initiation of discontinuous yielding were studied. As the

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temperature is increased above 4 K, discontinuous yielding begins at higher stresses and strains; discontinuous yielding is not present at temperatures above 30 K. Results are interpreted in terms of macroscopic heat balances and localized generation of heat from moving dislocations.

PB91-194795
Not available NTIS
National Inst. of Standards and Technology (NML),
Boulder, CO. Chemical Engineering Science Div.
High-Temperature Thermal Properties of UNS
\$44004 Using Multivariant Applications. S44004 Using Multivariant Analysis. Final rept.

L. J. Freiberger, and J. W. Bransford. 1990, 10p Sponsored by National Aeronautics and Space Admin-istration, Huntsville, AL. George C. Marshall Space

Pub. in Advanced Earth-to-Orbit Propulsion Technology 1990, vI p113-122.

Keywords: \*Stainless steel-440, \*Liquid metals, \*Combustion, Thermophysical properties, Mathematical models, Melting points, Thermal conductivity, Extrapolation, Thermodynamic properties, Spacecraft construction materials, Multivariate analysis, High temperature tests. Provides ature tests, Reprints.

In order to model the thermal behavior of steel alloys in the temperature range at which ignition and combus-tion may occur, their thermophysical properties at temperatures up to their melting points, approximately 1600 to 1800 K for many iron, nickel and cobalt-based alloys, must be known. Published values of thermal conductivity, specific heat, and emissivity are either given for much lower temperatures or are absent for alloys of special interest. Therefore, the development of a simple experimental method coupled with a numerical technique that can be used to extrapolate existing data or to estimate property values where no data exists was undertaken. The paper describes the experiment and numerical technique. The application of the procedures to estimate the thermophysical properties of UNS S44004 (AISI 440-C) are discussed.

101,161
PB91-195321
National Inst. of Standards and Technology (IMSE),

Rational list. of Standards and Technology (Index), Gaithersburg, MD. Polymers Div. Rate of Pyrite Bioleaching by 'Thiobacillus fer-rooxidans': Results of an Interlaboratory Comparison.

Pub. in Applied and Environmental Microbiology 57, n3 p642-644 Mar 91.

Keywords: \*Pyrite, \*Beneficiation, \*Leaching, \*Biotechnology, Standards, Iron, Extractive metallurgy, Interlaboratory comparisons, Rates(Per time), Variability, Thiobacillus ferroxidans, Variability, Reprints.

Ten laboratories participated in an interlaboratory Ten laboratories participated in an interlaboratory comparison of determination of bioleaching rates of a pyrite reference material. A standardized procedure and a single strain of Thiobacillus ferrooxidans were used in the study. The mean rate of bioleaching of the pyrite reference material was 12.4 mg of Fe per liter per h, with a coefficient of variation (percent relative standard deviation) of 32% as determined by eight laboratories. Those secults show the procession among laboratories. oratories. These results show the precision among lab-oratories of the determination of rates of pyrite bio-leaching when a standard test procedure and reference material are used.

101,162 PB91-195404 Not available NTIS

Notional Inst. of Standards and Technology (IMSE), Gaithersburg, MD. Polymers Div.
Characterization by High Performance Liquid Chromatography (HPLC) of the Solubilization of Phosphorus in Iron Ore by a Fungus. Final rept.

E. J. Parks, G. J. Olson, F. E. Brinckman, and F.

Baldi. 1990, 7p Pub. in Jnl. of Industrial Microbiology 5, n2-3 p183-189

Keywords: \*Biotechnology, \*Fungi, \*Liquid column chromatography, \*Iron, \*Phosphorus, \*Beneficiation, Contamination, Characterization, Leaching, Metalliferous ores, Apatites, Hydroxy compounds, Solvation, Oxalic acid, Metabolites, Solubilization, Hydrochloric acid, Separation processes, Reprints.

The value of iron ore is adversely affected by phosphorus in concentrations over 0.03 percent by weight. The

present research concerns using metabolic products of fungi to leach insoluble phosphates (hydroxyapatite) from ores. Ion chromatography was used to measure metabolization of glucose into acidic fragments. The rate and products of glucose degradation depend on both the chemical composition of the growth medium (buffered or not) and incubation conditions (shaken or quiescent). The principal products are identified as oxalic acid and tautomers of propylene dicarboxylic acid, mainly itaconic acid. Slow metabolization of the latter generates more oxalic acid. Aliphatic acids were not detected. Both iron ore phosphate and calcium phosphate are partially solubilized by either the spent broth or aqueous oxalic acid. Solubilization of ore phosphorus is greatly assisted by hydrochloric acid added to the spent broth in small increments. The data suggest biological and chemical leaching procedures for iron ore dephosphorization.

101,163 PB91-195529 Not available NTIS National Inst. of Standards and Technology (MSEL), Boulder, CO. Fracture and Deformation Div. Nitrogen Strengthening of Austenitic Stainless

Steels at Low Temperatures.

Final rept.

R. P. Reed, and N. J. Simon. 1989, 9p
Sponsored by Department of Energy, Washington, DC.
Pub. in Proceedings of International Conference on
High Nitrogen Steels, Lille, France, May 18-20, 1988,
p180-188 1989.

Keywords: \*Austenitic stainless steels, \*Nitrogen, \*Yield strength, \*Stress relaxation, \*Low temperature, Hardening(Materials), Tensile properties, Mechanical properties, Stresses, Strains, Elastic properties, Re-

Additions of nitrogen to austenitic steels significantly increase their flow strengths at low temperatures. Tensile stress-strain, stress relaxation, and strain-ratechange measurements on Fe-Cr-Ni alloys have been completed. For these same alloys, elastic constants and lattice parameters were measured from 295 to 4 K. Regression analyses of NBS data was used to assess the dependence of yield strength on carbon and nitrogen content. These data were interpreted in terms of strengthening mechanisms.

PB91-236505 Not available NTIS National Inst. of Standards and Technology (MSEL), Boulder, CO. Materials Reliability Div. Spatially Overdetermined Analysis for Propagation Toughness Using Strain Gages.

Final rept.

Pub. in Mechanics Research Communications 17, n2 p93-99 1990.

Keywords: \*Strain gages, \*Toughness, \*Stainless steels, \*Fracture properties, Fracture tests, Fractures(Materials), Strain measurement, Mechanical properties, Crack propagation, Cracking(Fracturing), Spatial distribution, Reprints.

Recent work by the authors has shown the applicability of strain measurements to static and dynamic frac-ture characterizations. Here they develop a methodol-ogy to analyze the spatial variations in strain sensed by a series of strain gages as a crack propagates beneath them. They analyze the dynamic fracture of a 4340 steel compact specimen using the developed methodology. The propagation toughness was determined to be 119 MPa square root of m at a crack speed of 644

101,165 PB91-236943 Not available NTIS
National Inst. of Standards and Technology (MSEL),
Boulder, CO. Materials Reliability Div.
Load-Controlled Tensile Tooks

Load-Controlled Tensile Tests of Austenitic Steels at 4 K. Final rept.

H. M. Lee, R. P. Reed, and J. K. Han. 1990, 10p Sponsored by Department of Energy, Washington, DC. Pub. in Advances in Cryogenic Engineering (Materials), v36 p1273-1282 1990.

Keywords: \*Tension tests, \*Low temperature tests, \*Loads(Forces), \*Austenitic stainless steels, \*High strength steels, Tensile properties, Ultimate strength, Yield point, Fracture properties, Mechanical properties, Yield strength, Reprints.

Load-controlled tensile tests were conducted at 4 K on high-strength austenitic steels. The rate of loading was

varied from 5 to 5000 N/s. This change of loading rate affected the onset of discontinuous yielding and, in turn, the fracture characteristics of the steels. Ultimate strength decreased at higher loading rates. The role of discontinuous yielding in affecting the dependence of these properties on loading rate is discussed. If con-ventional pressure vessel codes are used for the designation of structural design stresses, these data suggest that the ultimate strength, not the yield strength, controls the assignment.

101,166 PB91-237081 Not available NTIS National Inst. of Standards and Technology (MSEL),

Boulder, CO. Materials Reliability Div.
Interlaboratory Tension and Fracture Toughness
Test Results for CSUS-JN1 (Fe-25Cr-15Ni-0.3N)
Austenitic Stainless Steel at 4 K.

Final rept. H. Nakajima, K. Yoshida, S. Shimamoto, R. L. Tobler, R. P. Reed, R. P. Walsh, and P. T. Purtscher. 1990,

Sponsored by Department of Energy, Washington, DC.

Office of Fusion Energy.
Pub. in Advances in Cryogenic Engineering (Materials), v36 p261-268 1990.

Keywords: \*Austenitic stainless steels, \*Low temperature tests, \*Fracture properties, \*Toughness, Fractures(Materials), Standards, Experimental data, Fracture tests, Mechanical properties, Cryogenics, Tension tests, Reprints.

Interlaboratory tests are part of the U.S.-Japan cooperative program in fusion energy to establish cryogenic test standards for structural alloys. The second round of 4-K tension and fracture toughness tests for CSUS-JN1 (Fe-25Cr-15Ni-0.35N) austenitic stainless steel are described in the paper. The scatter of interlaborations are second programs as the second resolution of the second resolution in the second resolution in the second resolution is considered to the second resolution in the second resolution in the second resolution in the second resolution in the second resolution is second resolution. tory measurements is acceptable if some fracture toughness data are excluded as outliers.

101.167 PB91-237206 Not available NTIS National Inst. of Standards and Technology (MSEL), Boulder, CO. Materials Reliability Div.

Effect of Processing on 4-K Mechanical Properties

of a Microalloyed Austenitic Stainless Steel. Final rept.

P. T. Purtscher, M. C. Mataya, L. M. Ma, and R. P. Reed. 1990, 8p Sponsored by Department of Energy, Washington, DC.

Office of Fusion Energy.

Pub. in Advances in Cryogenic Engineering (Materials), v36 p79-86 1990.

Keywords: \*Austenitic stainless steels, \*Toughness, \*Fracture properties, Tensile properties, Hot rolling, Alloy steels, Mechanical properties, Hot working, An-nealing, Cryogenics, Low temperature tests, Reprints.

Tensile and fracture toughness tests were performed at 4 K as a function of hot-rolling temperature and compared with similar data for the steel in the annealed condition. Results show that the properties in hot-rolled conditions were comparable to annealed steel so there was no advantage to annealing after processing. Microalloy precipitates were effective at controlling grain size during processing at temperatures below 1150 C, and did influence the flow stress at 4 K

101,168 PB91-237248 Not available NTIS Notional Inst. of Standards and Technology (MSEL), Boulder, CO. Materials Reliability Div. Strain Rate Effect on Tensile Properties at 4 K of a VAMAS Round-Robin Austenitic Steel.

Final rept.

Pub. in Advances in Cryogenic Engineering (Materials), v36 p1061-1068 1990.

Keywords: \*Tensile properties, \*Strain rate, \*High strength steels, \*Austenitic stainless steels, \*Low tem-perature tests, Ultimate strength, Mechanical tests, Mechanical properties, Tension tests, Yield point, Displacement, Reprints.

A high-strength austenitic steel with nominal composition Fe-25Cr-14Ni-0.37N was included in an international round-robin measurement program. Tensile and fracture toughness tests were conducted at 4 K by leading low temperature test laboratories in Japan, Europe, and the U.S. The paper reports on the effect

# Iron & Iron Alloys

of strain rate on displacement-controlled tensile tests at 4 K. Similar to other recent results on austenitic steels, a transition in ultimate strength was observed as a function of strain rate: at higher strain rates the strength decreased about 10%. The onset of discontinuous yielding was also strain-rate dependent. The reduction of ultimate tensile strength is associated with the change from the nucleate to film heat transfer mechanism from the specimen surface to liquid helium.

101,169

PC A03/MF A01 PB92-108901 National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Metallurgy Div.

Mechanical Properties and Fracture Toughness of AAR TC128 Grade B Steel in the Normalized, and Normalized and Stress Relieved Conditions

G. E. Hicho, and D. E. Harne. Sep 91, 46p NISTIR-4660, REPT-24

See also PB90-207796.

Keywords: \*Fracture mechanics, \*Toughness, \*Carbon steels, \*Fracture strength, Tensile strength, Keywords: Normalizing(Statistics), Stress relaxation, Temperature dependence, Crack opening displacement, Manganese alloys, Tank cars, Jintegral

Traditional mechanical property tests, ultimate and yield strength, reduction in area, elongation, impact, and the nil-ductility temperature were performed on AAR TC128 grade B steel in the normalized, and the normalized and stress relieved conditions from -51 C to room temperature. In addition the crack initiation fracture toughness, as function of temperature, was determined using crack tip opening displacement (CTOD) and J integral test procedures. The crack arrest fracture toughness, as a function of temperature were also determined. It was found that the normalized and stress relieved steel had overall better mechanical and fracture toughness properties than the normalized

101.170

PB92-116615 Not available NTIS National Inst. of Standards and Technology (MSEL), Boulder, CO. Fracture and Deformation Div.

Ultrasonic Measurement of Sheet Steel Texture and Formability: Comparison with Neutron Diffraction and Mechanical Measurements.

Final rept. A. V. Clark, R. B. Thompson, Y. Li, R. C. Reno, G. V. Blessing, D. V. Mitrakovic, R. E. Schramm, and D.

Matlock, 1990, 19p
Pub. in Research in Nondestructive Evaluation 2, p239-257 1990.

Keywords: \*Steels, \*Metal sheets, \*Ultrasonic tests, Rolling, Nondestructive tests, On-line measurement systems, Plastic deformation, Electroacoustic transducers, Predictions, Measurement, Orientation, Comparison, Neutron diffraction, Formability, Texture, Lamb waves, Reprints, Orientation distribution coefficients, R-value.

Ultrasonic measurements were made on a set of thin steel sheets, using the lowest-order shear horizontal mode (SH(sub 0)-mode) and lowest-order symmetric Lamb-wave mode (S(sub 0)-mode). The velocities of these modes were measured as a function of angle relative to the sheet rolling direction. From the data reduction it is, in theory, possible to (1) partially characterize the texture of the sheet, and (2) predict the plastic strain ratio (r-value). The plate texture can be completely characterized by quantities known as orientation distribution coefficients (ODCs). The lowest-order ODCs can be obtained from the measurements; these were compared with ODCs measured by neutron diffraction, with good agreement for the dominant ODC. The r-value is a commonly used measure of sheet formability. It is typically measured mechanically with uniaxial tension specimens subjected to large plastic strain. Therefore, the r-value test is destructive and time consuming. A good correlation was found between S(sub 0)0mode velocity measurements and the average in-plane r-value. Consequently, the use of noncontacting electromagnetic-acoustic transducers (EMATs) may offer an online nondestructive measurement of sheet formability.

101,171 PB92-126515 PC A07/MF A02 National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Metallurgy Div.

Metallurgy Division, Technical Activities 1991. (NAS-NRC Assessment Panel February 13-14,

1992). Annual rept. 1 Oct 90-30 Sep 91. E. N. Pugh, and S. C. Hardy. Dec 91, 136p NISTIR-

See also PB91-132225

Keywords: \*Metallurgy, \*Research projects, Metal matrix composites, Alloys, Superconductors, Corrosion, Electrodeposition, Magnetic materials, Mechanical properties, Process control, Intermetallic alloys, Metals processing, Process sensors.

The report summarizes the FY 1991 activities of the Metallurgy Division of the National Institute of Standards and Technology (NIST). These activities center upon the structure-processing-properties relations of metals and alloys and on methods of measurement; and also include the generation and evaluation of critical materials data. Efforts comprise studies of metals processing and process sensors; advanced materials, including metal matrix composites, intermetallic alloys and superconductors; corrosion and electrodeposition; mechanical properties; magnetic materials; and high temperature reactions.

## Lubricants & Hydraulic Fluids

PB91-158808 Not available NTIS National Bureau of Standards (IMSE), Gaithersburg, MD. Ceramics Div.

Mechanisms of Additive Effectiveness.

Final rept. S. M. Hsu, P. Pei, C. S. Ku, R. S. Lin, and S. T. Hsu.

1986, 10p Sponsored by Department of Energy, Washington, DC. Pub. in Proceedings of International Colloquim Additives for Lubricants and Operational Fluids (5th), January 14-16, 1986, p3.14-1-3.14-10

Keywords: \*Lubricant additives, \*Wear, \*Tribology, Oxidation, Corrosion, Fluid-solid interactions, Reaction kinetics, Polar compounds, Reprints.

The interactions among naturally occurring polar mo-lecular species with additives in wear and oxidation are studied. Base oil hetroatoms such as sulfur, nitrogen, and oxygen have pronounced effects on additive performance. Interaction studies in wear and oxidation tests suggest a complex chemical reaction mechanism that has heretofore been little understood but is beginning to be defined now by critical experiments.

101.173

PB91-158923 Not available NTIS National Inst. of Standards and Technology (IMSE), Gaithersburg, MD. Ceramics Div. Heats of Immersion, Friction, and Wear of Base Oil

Final rept. F. E. Lockwood, K. Bridger, and S. M. Hsu. 1989,

Pub. in Tribology Transactions 32, n4 p506-516 1989.

Keywords: \*Lubricating oils, \*Mixed base crudes, Friction, Adsorption, Surface chemistry, Thermodynamic properties, Fluid flow, Wear, Interfacial tension, Reprints, \*Heat of immersion.

Heats of immersion were determined for three base oils, their fractions as separated by polarity, and model compounds on a 52,100 steel surface. The method consists of calculating the heat of immersion based on surface tension and contact angle measurements made at temperatures from 25C to 175C. Friction and wear tests were performed on the same oils using micro-sample four-ball wear tests. The heat of immersion data were found to be inversely proportional to friction and wear. Model compounds with different functional groups similarly tested, however, suggest molecular structures have a significant role in influencing friction and wear when chemical reactions become the dominant lubrication mechanism rather than adsorption.

101,174

PB91-174862 Not available NTIS National Inst. of Standards and Technology (IMSE), Gaithersburg, MD. Ceramics Div.

Mechanisms of Additive Effectiveness. Final rept.

S. M. Hsu, P. Pei, C. S. Ku, R. S. Lin, and S. T. Hsu.

1989, 20p Sponsored by Department of Energy, Washington, DC. Pub. in Lubrication Science 1, n2 p165-184 Jan 89.

Keywords: \*Lubricant additives, \*Tribology, Interactions, Lubricating oils, Wear, Oxidation, Quantity ratio, Calorimetry, Mechanism, Reprints, FRT, ZDP, Four-

The article discusses the nature and extent of base oiladditive and additive-additive interactions. The first interaction is in the bulk oil phase, where solution chemistry is involved. The second interaction occurs at the wear surfaces. Various experimental techniques (DSC, thin film oxygen uptake, FRT, four ball) were used to measure interactions. In an examination of base oil-additive-interactions on oxidation stability, various species of base oils exert a strong influence on the performance of antioxidants. In additive-additive interactions, the data suggest a strong concentration of dependent interaction patterns among the various additives and the base oils. Mechanistic studies are recommended to elucidate some of the observed phenonema.

101,175 PB91-174953 Not available NTIS National Bureau of Standards (IMSE), Gaithersburg,

MD. Ceramics Div. Study of Additive Response in a Series of Rerefined Base Oils Typical of Current Commercial

Practice. Final rept.

Pub. in Proceedings of European Tribology Congress (4th), Ecully, France, September 9-12, 1985, v1 p1-13.

Keywords: \*Automobiles, \*Lubricating oils, \*Tribology, Lubricant additives, Compositions, Refining, Oxidation, Comparison, Recycled materials, Thin films, Reprints, Oxygen uptake.

A group of 14 rerefined base oils representing 6 refining processes and 10 geographic areas of the U.S. and Canada have been evaluated extensively to determine compositional detail. The additive responses of these compositional detail. The additive responses of these base oils to six commercial automotive additive packages were studied. The NBS thin film oxygen uptake test (TFOUT) was used in the study with test conditions which showed good correlation with IIID engine sequence test results. A group of 43 virgin base oils with a common additive package was also tested for comparison with the rerefined base oils. The oxidation induction times from the TFOUT with six commercial additive packages were correlated with basestock compositional parameters. The study shows that satisfactory quality commercial motor oils can be formulatfactory quality commercial motor oils can be formulat-ed with rerefined base oils and a number of commer-cial additive packages. Correlational studies show that the major compositional parameters that are important with rerefined oils are sulfur, nitrogen, and polars, all of which have a negative effect on additive response.

101,176

PB91-189407 Not available NTIS National Inst. of Standards and Technology (IMSE), Gaithersburg, MD. Ceramics Div. Study on the Nature of Boundary Lubricating Film:

Analytical Method Development Final rept.

R. S. Gates, S. M. Hsu, and K. L. Jewett. 1989, 8p Sponsored by Department of Energy, Washington, DC. Energy Conversion and Utilization Technologies Div. Pub. in Tribology Transactions 32, n4 p423-430 1989.

Keywords: \*Tribology, \*Lubrication, \*Polymeric films, \*Chemical analysis, \*Fluid-solid interactions, Refractivity, Organometallic compounds, Ultraviolet spectra, Absorption spectroscopy, Molecular weight, Surface chemistry, Interfaces, Oxidation, Wear, Reprints, Size exclusion chromatography.

The nature of the boundary lubricating film and its formation mechanism has been the subject of research in the last several decades. The study describes the development of a novel analytical technique designed specifically for the analysis of small amounts of lubricating film using an integrated size exclusion chromatography-refractive index-ultraviolet-graphite furnace atomic absorption (SEC-RI-UV-GFAA) system. Experiments under static simulation conditions as well as under dynamic rubbing conditions were conducted.

# Lubricants & Hydraulic Fluids

Analysis of the reaction products in each case indicates the formation of high molecular weight organometallic compounds with molecular weights range from 1,000 to 100,000. The paper describes the methodology, equipment, and the procedures developed to measure nanogram quantities of the organometallic compounds generated by the tribochemical reactions in the boundary contact of a four ball wear tester.

101,177 PB91-189480 Not available NTIS
National Inst. of Standards and Technology (IMSE),
Gaithersburg, MD. Ceramics Div.
Mechano-Chemical Description Mechano-Chemical Descriptive Model for Wear Under Mixed Lubrication Conditions.

Final rept. S. M. Hsu, E. E. Klaus, and H. S. Cheng. 1988, 17p Sponsored by Department of Energy, Washington, DC. Office of Basic Energy Sciences. Pub. in Wear 128, n3 p307-323, 15 Dec 88.

Keywords: \*Tribology, \*Lubrication, \*Wear, \*Surface chemistry, Probabilistic estimation, Performance prediction, Process control, Reprints.

The processes of lubrication are systematically analyzed and explained with the aid of recent experimental discoveries. Effective lubrication often involves surface chemical reactions which are dependent on contact geometry, load, speed, and environmental influences. Materials properties such as hardness, elasticity and others also affect the wear outcome. Fluid mechanics under the influence of interfacial pressures and temperatures control a significant portion of the wearing processes. A conceptual model is proposed to link all these factors in a line of defense framework, and to discuss how wear can be predicted based on a probabilistic model. The model proposes a series of criteria for various combinations of chemically controlled, and materials properties controlled situations.

101,178 PB91-195412 Not available NTIS National Inst. of Standards and Technology (IMSE), Gaithersburg, MD. Ceramics Div.

Diesel Deposit Forming Tendencies - Microanalysis Methods.

Final rept.

J. M. Perez, P. Pei, Y. Zhang, and S. M. Hsu. 1991, 10p

Sponsored by Department of Energy, Washington, DC. Pub. in SAE Technical Paper Series 910750 International Congress and Exposition, Detroit, MI., February 25-March 1, 1991, p1-10.

Keywords: \*Lubricants, \*Liquids, \*Diesel engines, \*Deposits, \*Tribology, Thermal degradation, Oxidation, Automotive engineering, Chemical analysis, Wear tests, Microanalysis, Reprints.

Liquid lubricants are cruicial to the successful develop-ment of advanced engines for the next decade. En-gines are being optimized to meet emission standards as well as improved durability and fuel economy. Lubricant research is focused on the severe environment and temperature requirements of advanced engines with a top ring reversal temperature of over 400 C. paper describes key lubricant considerations including oxidation and thermal stability, volatility, deposit formation, friction and wear control. Cooperative research efforts between industry and NIST resulted in several candidate high temperature liquid lubricants.

101,179 PB91-203810 Not available NTIS

Not available NTIS
National Inst. of Standards and Technology (MSEL),
Gaithersburg, MD. Ceramics Div.
Characterization of Tricresylphosphate Lubricating Films by Micro-Fourier Transform Infrared Spectroscopy. Final rept.

J. M. Perez, C. S. Ku, P. Pei, B. E. Hegemann, and

S. M. Hsu. 1990, 9p Pub. in Tribology Transactions 33, n1 p131-139 1990.

Keywords: \*Lubricant additives, \*Films, \*Tribology, \*TCP, Infrared spectra, Fourier transformation, Characterization, Microanalysis, Wear tests, Calorimetry, Oxidation, Temperature dependence, Corrosion products, Chemical analysis, Methodology, Reprints.

The characterization of tricresylphosphate lubricating films by use of micro-Fourier Transform Infrared Spectroscopy is reported. The study uses a combination of test methods to establish the sequence of chemical reactions that result in the formation of anti-wear films

observed. A four-ball wear test sequence, using a 6 microliter sample to increase test severity, generated the tribological films. A pressurized differential scan-ning calorimeter (DSC) was used to obtain oxidized samples at various temperatures. The wear contact temperatures are estimated by comparison of the spectra analyses of the oxidation products to the wear film analyses. The combination of test methods is rapid and reliable. DSC oxidation and spectra analyses coupled with the sequential wear test method enabled characterization of the films formed. The approach is useful in evaluating additive effectiveness.

PB91-236711 Not available NTIS National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Ceramics Div.

Effect of Selected Chemical Compounds on the Lubrication of Silicon Nitride.

Final rept. R. S. Gates, and S. M. Hsu. 1991, 9p Sponsored by Department of Energy, Washington, DC. Energy Conversion and Utilization Technologies Program. Pub. in Tribology Transactions 34, n3 p417-425 1991.

Keywords: \*Tribology, \*Lubricant additives, \*Ceramics, \*Friction, \*Wear tests, \*Paraffin, \*Silicon nitrides, Sulfonic acids, Monomolecular films, Oleic acid, Salicylic acid, Imidazoles, Phenol, Lubricating oils, Fluidsolid interactions, Phosphorus compounds, Glycols,

Information on the chemical interactions of ceramics is scarce. This is especially true for chemical interactions with regard to lubrication of these materials. The paper investigates the influence of selected chemical compounds on the friction and wear of silicon nitride under boundary lubrication conditions. A ball-on-three-flat modification of the four-ball wear tester was utilized to evaluate the tribological characteristics of a hot pressed silicon nitride lubricated with a paraffinic base oil containing 1 weight percent additives. Friction, wear, and film formation tendencies were observed for a range of oil soluble chemical compounds containing oxygen, sulfur, nitrogen, chlorine, and phosphorus. A wide range of additive response was observed. Friction coefficient varied from increases of 30 percent to decreases of 47 percent below that of the base case of paraffin oil without additive. Wear was measured as the wear scar diameter increase above the Hertz diameter. Relative to the base case, wear additive response ranged from an increase in diameter of 61 percent to a decrease of 96 percent. Successful wear reduction was obtained by all phosphorus containing com-pounds, several glycol compounds, oleic acid, sulfon-ates, a salicylate, an imidazoline, and a phenol, and was generally associated with the formation of a film in the contact region.

# **Materials Degradation & Fouling**

*101,181* PB91-143313 PC A03/MF A01 National Inst. of Standards and Technology (IMSE), Gaithersburg, MD. Polymers Div.
Studies on the Degradation Products of Paper with and without Pollutants in a Closed Environment. 1.

Preliminary Results.

E. J. Parks, C. M. Guttman, K. L. Jewett, and F. E. Brinckman. Dec 90, 47p NISTIR-4456
Sponsored by National Archives and Records Administration, Washington, DC.

Keywords: \*Newsprint, \*Papers, \*Degradation, \*Sulfur dioxide, \*Acetic acid, Aging tests(Materials), Organic acids, Gas chromatography, Mass spectroscopy, Liquid chromatography, Graphs(Charts).

The authors have developed methods using Mass Spectroscopy, Liquid Chromatography and Gas Chromatography to detect degradation products of rag paper and newsprint in the presence of some common air pollutants. They have searched for products that might themselves be autocatalytic to encourage degradation of these materials. In particular, they have looked at gaseous degradation products and those degradation products which are mobile and which may be transferred one paper to another by surface or gas phase diffusion. Six organic acids have been tentatively identified as degradation products which are surface

mobile on newsprint and rag paper. Acetic acid is a major organic acid gas phase component. The results of these studies were correlated with more traditional bulk paper properties tests.

101,182

PB91-144345 PC A03/MF A01 National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Polymers Div.

Synthesis of Prototype Resins for Use as BEP Intaglio Ink Vehicles Curing by Electron Beam Radiation.

Annual rept.

B. J. Bauer, and B. Dickens. Dec 90, 45p NISTIR-4474

Sponsored by Bureau of Engraving and Printing, Washington, DC.

Keywords: \*Radiation curing, \*Resins, \*Electron beams, \*Inks, X ray analysis, Neutron scattering, Chemical radiation effects, Polymeric films, Transition temperature, Polymethyl methacrylate, Copolymers, Polyoxyethylene, \*Intaglio ink.

Macromonomers have been investigated as components in electron beam curing resins for use in intaglio inks. Thermal studies of cured samples of macromonomer-conventional monomer networks show a single transition for macromonomer containing samples and multiple transitions for equivalent samples made with unfunctionalized polymer. Small angle neutron and xray scattering studies show that samples made with macromonomers are much more uniform than those made with unfunctionalized polymers. Cure studies show that macromonomers with different polymerizable end groups have very different rates of cure, most of the groups inhibiting the cure.

101 183

PB91-159269 Not available NTIS National Bureau of Standards (IMSE), Gaithersburg,

MD. Metallurgy Div.

Method for Quantitative Measurement of Galling Damage.

Damage.
Final rept.
E. P. Whitenton, M. B. Peterson, and L. K. Ives.
1987, 16p
Pub. in Proceedings of Metal Transfer and Galling in
Metallic Systems Symposium, Orlando, FL., October
8-9, 1986, p155-170 1987.

Keywords: \*Galling, \*Tribology, \*Metals, Quantitative analysis, Measurement, Damage assessment, Profilometers, Sensor mapping, Surface roughness, Wear, Computerized simulation, Reprints.

Galling damage at sliding contacts is recognized by the occurrence of a significant increase in surface roughness, characterized by gouges, grooves, prows, transferred lumps of material, and sometimes cracks. In the past, little effort has been made to measure the severity or nature of the damage quantitatively. Rather, a description based on visual observation was usually the only means employed to distinguish between the damage produced by different tribological contact conditions or exhibited by different types of materials. The method described employs an automated profilometer system to map a relatively large area of the damaged surface. From the topographic data obtained it was possible to evaluate parameters that are descriptive of the area as a whole rather than along a single trace as is normally done in profilometer based roughness measurements. Three rather simple parameters were found to give a good account of observed galling damage. The parameters were the average maximum peak to valley roughness, Rt ave., the displaced volume, DV, and a measure of the shape or aspect ratio of damage feature, AR. Results using these and other parameters are given. In addition, different galled surfaces are compared using computer generated damage maps.

101,184

PB91-174904 Not available NTIS National Inst. of Standards and Technology (IMSE), Gaithersburg, MD. Ceramics Div. ACTIS: Towards a Comprehensive Tribology Data

Base.

S. Jahanmir, S. M. Hsu, and R. G. Munro. 1989, 9p Pub. in Computerization and Networking of Materials Data Bases, ASTM STP 1017, p340-348 1989.

# Materials Degradation & Fouling

Keywords: \*Data bases, \*Tribology, International co-operation, Technology transfer, Friction, Lubrication, Wear, Design criteria, Reprints, \*Actis code.

Tribology is being increasingly recognized as a critical discipline that can play a key role in raising the level of U.S. competitiveness. The transfer of tribology research information into general engineering practice can be made quickly and efficiently by the computerizing of tribology data. The tribology community has been participating in an international effort to centralize and computerize tribology data that goes beyond the establishment of bibliographic data bases. The community is developing a computerized tribology information system as a self-sustaining activity, with gov-ernment providing the initial funding for research and prototype construction of a PC-based system that contains six data-base components: numeric, design, newsletter, research-in-progress, bibliography, and product and services directory. The numeric data base, which contains 'best judgment' values compiled by experts, and the design data base, which contains validated design programs, are being developed in the first two years of a six-year program. These two data bases present a formidable technical challenge, since not only must they be self-contained, but they must also interact.

Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Inorganic Analytical Research Div. Method to Enhance Porosity of Micro-particles.

Final rept. B. S. Carpenter, L. C. Sander, C. Horvath, and W. R.

Brown. 1988, 9p Pub. in Jnl. of Radioanalytical and Nuclear Chemistry 124, n2 p523-531 1988.

Keywords: \*Silica, \*Fission products, \*Uranium, \*Porosity, \*Ceramics, Coatings(Materials), Trace elements, Fission tracks, Microparticles, Reprints

The Nuclear Track Technique (NTT) is used to enhance the porosity of silica micro-particles. The enhanced porosity is a result of the formation of surface and interior pores or tracks in the silica by the action of external and internal fission fragments. The fission tracks produced at the surface and within the interior of the micro-particles are a result of coating the particles with trace quantities of uranium, instead of having trace quantities of uranium incorporated within the silicon dioxide matrix.

101,186 PB91-189530 Not available NTIS National Inst. of Standards and Technology (IMSE), Gaithersburg, MD. Ceramics Div.

Tribological Characteristics of Synthesized Diamond Films on Silicon Carbide. Final rept.

S. Jahanmir, L. K. Ives, A. Feldman, E. Farabaugh, and D. E. Deckman. 1989, 9p Pub. in Wear 133, n1 p73-81 1989.

Keywords: \*Tribology, \*Vapor deposited coatings, \*Diamonds, \*Silicon carbides, \*Ceramics, \*Wear, X ray analysis, Friction, Surface chemistry, Thin films, Graphite, Reprints, Carbon films.

The purpose of the research is to explore the possible use of synthesized diamond films as wear resistant, low friction materials for tribological applications. Silicon carbide specimens, in the form of small disks, were coated with diamond films using the hot filament CVD process. A ball-on-three-flat contact geometry was used in the wear experiments. The experimental results confirmed that wear rate of the disk specimens can be reduced by a factor of 200, when they are deposited with a diamond film. The fraction coefficient was reduced by almost one order of magnitude. Although it was not explicitly shown the wear resistance may be related to the hardness of the diamond film. EDAN analysis of the worn surface of the diamond in-dicated that the SiC counterface undergoes tribochemical reactions with the air atmosphere producing hydrated silicates. Formation of the tribochemical reaction product cannot be responsible for low friction coefficients, since the same material is formed in SiC/ SiC tests. It is, therefore, hypothesized that the low friction coefficient of diamond may be related to formation of a thin film of graphite at the real area of contact. Removal of these graphitic regions by wear would then produce a smooth wear surface.

101,187 PB91-190017

Not available NTIS

National Inst. of Standards and Technology (IMSE), Gaithersburg, MD. Ceramics Div.

Comparison of Standard Test Methods for Non-Lubricated Sliding Wear.

Final rept. A. W. Ruff. 1989, 9p Pub. in Wear 134, n1 p49-57 1989.

Keywords: \*Standards, \*Interlaboratory comparisons, \*Wear tests, \*Tribology, Sliding friction, Methodology, Variability, Metals, Solid-solid interfaces, Reprints.

The paper analyzes non-lubricated sliding wear data obtained using three standard test methods and ge-ometries: block-on-ring, crossed-on-cylinder, and pin-on-disk. The data discussed here were obtained in interlaboratory testing programs where the conditions were carefully specified, and where the test materials were provided to the different laboratories. Such an approach should provide the most consistent data and should allow direct comparison of the intrinsic characteristics of the different test methods. However, results showed that when the above mentioned three tests were carried out under similar load and speed conditions, the typical within-laboratory variation in reproducing wear volume measurements in metal-on-metal sliding ranged from 21% to 57%. By comparison, using standard test methods one finds the variation to be about 5% for abrasive wear, and about 5% for erosive wear.

PB91-190025 Not available NTIS National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Ceramics Div. Sliding Wear Studies of Nickel-Copper Composi-

tion-Modulated Coatings on Steel. Final rept.

A. W. Ruff, and Z. X. Wang. 1989, 14p Pub. in Wear 131, n2 p259-272 1989.

\*Tribology, \*Wear tests, occur, alloys, \*Copper alloys, alterials), \*Nickel alloys, \*Compositions alloys, Composi-\*Coatings(Materials), \*Nickel alloys, \*Copper alloys, Friction alloys, Sliding friction, Binary alloys, Compositions, Laminates, Loads(Forces), Reprints.

Sliding wear measurements have been conducted on Ni-Cu composition-modulated coatings on steel. The coatings consisted of alternate layers of nickel and copper with layer spacings of 10 nm and 100 nm. Pure nickel and pure copper coatings were also prepared in the same way and studied. The coated steel cylinders were slid against 52100 steel in a crossed-cylinder test under clean conditions without lubrication at various loads and sliding distances. It was found that the most wear-resistant coating was the one having the smalllow loads. Both composition-modulated coatings showed less wear than coatings of pure Cu and Ni from the same solution. The layer microstructure in these coatings is believed to provide internal barriers to wear damage that lead to the improvements in wear resistance. Results from examination of the worn specimens and collections of wear debris are also described

### Miscellaneous Materials

PB91-147074 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Thermophysics Div.
Alternative Refrigerants R123a, R134, R141b, R142b, and R152a: Critical Temperature, Refrac-

tive Index, Surface Tension, and Estimates of Liquid, Vapor, and Critical Densities. Final rept.

H. B. Chae, J. W. Schmidt, and M. R. Moldover. 1990, 6p

Sponsored by Department of Energy, Washington, DC. Pub. in Jnl. of Physical Chemistry 94, n25 p8840-8845, 13 Dec 90.

Keywords: \*Refrigerants, Critical temperature, Critical density, Refractive index, Interfacial tension, Surface tension, Reprints, Chlorofluorocarbons.

Differential capillary rise and refractive index data are reported for five alternative refrigerants: R123a(CHCIF-CCIF2), R132(CHF2-CHF2), R141b(CCIF2-CH3), The data extend from about 25 C to the critical point of each fluid and directly yield the critical temperature Tc and the temperature-dependent capillary length. The present data were combined with liquid density data (near ambient temperature) to determine the Lorentz-Lorenz constant. The Lorentz-Lorenz relation is used to estimate the liquid, vapor, and critical densities, and the surface tension.

101.190

PB91-149344 Not available NTIS National Bureau of Standards (IMSE), Gaithersburg, MD. Ceramics Div.

Tensile-Fracture Resistance Mechanisms in Brittle Polycrystals: An Ultrasonics and In-situ Microscopy Investigation. Final rept.

P. L. Swanson, 1987, 22p

Contract USGS-414274 Sponsored by Geological Survey, Menlo Park, CA. Pub. in Jnl. of Geophysical Research-Solid Earth and Planets 92, nNB8 p8015-8036 1987.

Keywords: \*Brittle materials, \*Polycrystals, \*Fracture mechanics, Ceramics, Microscopy, Ultrasonic tests, Granite, Aluminum oxide, Rocks, Reprints, In-situ

The material-breakdown processes associated with mode-I fracture propagation in brittle polycrystals is investigated using ultrasonic-wave probing and in-situ optical microscopy. Emphasis is placed on delineation of the size and shape of the 'fracture process zone' and identification of its constitutive micromechanisms. Two materials were investigated: imperfectly-elastic multi-phase Westerly granite and near perfectly-elastic single-phase polycrystalline alumina (Al2O3). In both materials a zone of 'tractions' was observed to develop along the macrocrack flanks behind the visually-identified primary fracture tip. The tractions, or re-straining forces, were provided by both frictional interlocking of the fracture surfaces and 'bridging' by intact material left behind the advancing fracture front. Localized microcracking (friction-induced microcracking and material-bridge rupture) was found to be associated with the traction sites. Traction-zone lengths in the granite were as long as 15-40 mm (0.75 mm grain size) and 2 mm in the alumina (20-100 micrometer grain size). The crack-interface restraining mechanisms are incorporated into a simple fracture mechanics formulation which is used to describe several commonly observed features (e.g. R-curves) of macroscopic fracture behavior.

101.191

PB91-159137 Not available NTIS National Bureau of Standards (IMSE), Gaithersburg,

International Co-operation: The Versailles Project on Advanced Materials and Standards. Final rept.

L. H. Schwartz, and B. W. Steiner. 1988, 2p Pub. in ATAS Bulletin 5, p135-136 May 88.

Keywords: \*International cooperation, \*Materials, \*Standards, Reprints, \*VAMAS Project.

The formation and activity of the Versailles Project on Advanced Materials and Standards (VAMAS) is described.

101,192

PB91-159145 Not available NTIS National Bureau of Standards (IMSE), Gaithersburg,

VAMAS Bulletin. Final rept.

. H. Schwartz, and B. W. Steiner. Jul 87, 16p Pub. as VAMAS Bulletin, n6 p1-16 Jul 87.

Keywords: \*Materials, \*Standards, \*International co-operation, Reprints, \*VAMAS project.

Recent work of the Versailles Project on Advanced Materials and Standards (VAMAS) is described.

101.193

PB91-162024 Not available NTIS National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Polymers Div. Effect of Pyrophosphate Concentrations on Calcium Phosphate Growth on Well-Crystallized Octa-calcium Phosphate and Hydroxyapatite Seed Crystals.

Final rept.

N. Eidelman, W. E. Brown, and J. L. Meyer. 1991, 9p Sponsored by American Dental Association Health Foundation, Chicago, IL. Pub. in Jnl. of Crystal Growth 108, p385-393 1991.

Keywords: \*Calcium phosphates, \*Pyrophosphates, Crystal growth, Concentration(Composition), Apatites, Hydroxy compounds, Inhibitors, Comparison, Dental materials, Reprints.

The comparative effects of 0.3, 1 and 3 micromolar P2O7(sup 4-) concentrations on the growth of calcium phosphate on octacalcium phosphate (OCP) and on well-crystallized' hydroxyapatite (OHAp) seeds were studied. The control growth rates (without P2O7(sup 4-) were adjusted by weight or surface area of the seed crystals. The induction periods were longer with higher P2O7(sup 4-) concentrations and longer on OCP seeds than on the OHAp seeds. However, the final growth rates were about the same on both kinds of seeds when equal concentrations of P2O7(sup 4-) were used, suggesting that the same phase was growing on both kinds of seeds. The growth rates were faster when higher concentrations of OHAp seeds were used. The crystal growth on both OCP and OHAp seeds was accelerated when most of the labeled P2O7(sup 4-) disappeared from the solution. The composition of the initial phase that grayen either OCP are position of the initial phase that grew on either OCP or OHAp seed crystals appears to be OCP or partially hydrolyzed OCP. These results lead to the conclusion that apparently OCP, but not OHAp, grew on OCP and OHAp seeds in the presence of P2O7(sup 4-).

101,194 PB91-174243 PB91-174243 Not available NTIS
National Inst. of Standards and Technology (NEL),
Gaithersburg, MD. Building Environment Div.
Experimentation, Analysis, and Correlation of Refrigerant-22 Flow Through Short Tube Restrictors.
Final rent

Final rept.

D. A. Aaron, and P. A. Domanski. 1990, 13p Sponsored by Department of Energy, Washington, DC. Pub. in ASHRAE (American Society of Heating, Refrigerating and Air-Conditioning Engineers) Transactions, v96 pt1 13p 1990.

Keywords: \*Refrigerants, \*Pipe flow, \*Heat pumps, Tubes, Orifices, Air conditioners, Pressure reduction, Expansion, Diameters, Fluid flow, Mass flow, Reprints.

Refrigerant-22 flow through short tube restrictors was investigated. The analysis pertained to initially subcooled refrigerant flowing through short tubes with 5 <L/D < 20. The flow conditions studied were those typically found in heat pumps. Flow dependencies upon upstream subcooling, upstream pressure, downstream pressure, tube length, tube diameter, entrance cham-fering, and exit chamfering were examined. A correla-tion and flow charts for mass flow rate prediction were developed from a large experimental data base.

101,195 PB91-175414 Not available NTIS

Not available NTIS
National Inst. of Standards and Technology (NML),
Gaithersburg, MD. Thermophysics Div.
Thermodynamic Properties of Two Alternative Refrigerants: 1,1-dichloro-2,2,2-trifluoroethane
(R123) and 1,1,1,2-tetrafluoroethane (R134a). Final rept.

G. Morrison, and D. K. Ward. 1991, 22p Sponsored by Department of Energy, Washington, DC. Pub. in Fluid Phase Equilibria 62, p65-86 1991.

Keywords: \*Refrigerants, \*Thermodynamic properties, Temperature effects, Vapor pressure, Working fluids, Critical point, Thermophysical properties, Density(Mass/volume), Measurement, Pressure, Re-

The paper describes two different sets of measurements of the properties of two proposed alternative refrigerants, 1,1,2-tetrafluoroethane (R134a) and 1,1-dichloro-2,2,2-trifluoroethane (R123). The first are vapor-liquid equilibrium measurements made in a simple variable-volume sapphire cell. The vapor pressures and saturation liquid densities were determined for both materials, between 268 K and the critical temfor both materials, between 268 K and the critical temperature for R134a and between 303 K and 373 K for R123. The saturation vapor density was also determined for R134a from 298 K to the critical point, where the critical conditions were measured. The second set of measurements were made with a vibrating tube den-simeter from the saturation pressure to 5500 kPa for R134a and to 3500 kPa for R123 in the temperature range 278 K-368 K. These data are then compared with other determinations of similar properties.

101.196

Not available NTIS PB91-189563 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Building Environment Div. Study of Flow Boiling Heat Transfer with Refrigerant Mixtures.

Final rept.

D. S. Jung, M. O. McLinden, R. Radermacher, and D. A. Didion. 1989, 14p

Sponsored by Electric Power Research Inst., Palo Alto, CA.

Pub. in International Jnl. of Heat Mass Transfer. 32, n9 p1751-1764 1989.

Keywords: \*Heat pumps, \*Refrigerants, Heat transfer coefficient, Mixtures, Nucleate boiling, Reprints.

Mixture effects are studied on horizontal flow boiling heat transfer with both azeotropic and non-azeotropic refrigerant mixtures. More than 2000 local heat transfer coefficients are obtained with the azeotropic R12/ R152a mixture and compared against the previously measured data with the non-azeotropic R22/R114 mixture. In a convective evaporation region, small mass transfer resistance is found for mixtures. The variation of physical properties due to mixing is responsible for almost all of the heat transfer degradation. In a partial boiling region, however, severe degradation of heat transfer with mixtures, similar to that in nucleate pool boiling heat transfer with mixtures, is found. A suppression of nucleate boiling at lower qualities due to loss of wall superheat with mixtures is responsible for the degradation. An analysis is developed to pre-dict a transition quality by using Hsu's onset of nucle-ate boiling theory. The prediction agreed well with ob-served transition qualities for both pure and mixed refrigerants. Correlations, based on the supposition of Chen and using only phase equilibrium data to consider mixture effects, are developed with mean deviations of 7.2 and 9.6% for pure and mixed refrigerants.

101,197 PB91-236695 Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Thermophysics Div.

Thermodynamic Diagrams for Refrigerant Mixtures.

Final rept. J. S. Gallagher, M. O. McLinden, and G. Morrison.

1988, 18p Sponsored by Electric Power Research Inst., Palo

Pub. in ASHRAE (American Society of Heating, Refrigerating and Air-Conditioning Engineers) Transactions, v94 pt2 p2119-2136 1988.

Keywords: \*Refrigerants, \*Equations of state, \*Thermodynamic properties, Thermochemical diagrams, Fluorohydrocarbons, Entropy, Thermodynamics, Temperature, Pressure, Thermophysical properties, Thermochemical properties, Reprints, \*Thermodynamic diagrams

Several highly detailed diagrams of the thermodynamic properties of refrigerant mixtures have been generated. These diagrams are based on the Carnahan-Starling-DeSantis equation of state and are useful in the analysis and design of refrigeration equipment using refrigerant mixtures. Presented are pressure-enthalpy diagrams for R13/12, R22/114 and R22/11 mixtures at compositions of 60/40 and 40/60 weight percent for each mixture. Temperature-entropy dia-grams for the R22/114 mixture as well as for pure R22 and R114 are also presented. The CSD equation of state is briefly reviewed along with a description of the routines used to produce the diagrams.

101,198 PB92-112366 PC A05/MF A01

National Inst. of Standards and Technology (CSTL), Boulder, CO. Thermophysics Div. Survey of Current Worldwide Research on the Thermophysical Properties of Alternative Refrig-

erants.
M. O. McLinden, W. M. Haynes, J. T. R. Watson, and K. Watanabe. Jun 91, 82p NISTIR-3969
Prepared in cooperation with National Engineering

Lab., East Kilbride (Scotland), and Keio Univ., Yokohama (Japan). Dept. of Mechanical Engineering. Spon-

sored by Department of Energy, Washington, DC. Office of Buildings and Community Systems.

Keywords: \*Refrigerants, \*Thermophysical properties, Transport properties, Surveys, Research, Thermodynamic properties, Tables(Data), Fluorohydydrocarbons, Permittivity, Refractivity, Foreign technology, Global, Hydrochlorofluorocarbons, Hydrofluorocarbons.

The survey represents an exhaustive compilation of the research activities throughout the world concerned with either measurements or correlations of the ther-mophysical properties of alternative refrigerants. The properties covered in the study include thermodynamic, transport, phase equilibria, and other properties such as dielectric constant and refractive index. The survey has included a wide range of fluids (including R23, R32, R125, R143a, R22, R134a, R152a, R134, R124, R142b, R123, R123a, R141b) along with mixtures containing at least one of these fluids. The report presents in tabular form summary information about each research activity; the survey does not present raw data or correlating equations.

101,199

PB92-116748 Not available NTIS
National Inst. of Standards and Technology (NML),
Boulder, CO. Thermophysics Div.
Predictive Extended Corresponding States Model

for Pure and Mixed Refrigerants.

Final rept.

Pub. in Proceedings of ASHRAE-Purdue CFC and IIR-Purdue Refrigeration Conference, West Lafayette, IN., July 17-20, 1990, 10p.

Keywords: \*Thermophysical properties, \*Refrigerants, Enthalpy, Equations of state, Mixtures, Entropy, Thermal conductivity, Computer programs, Thermodynamic properties, Forecasting, Viscosity, Models, Density(Mass/volume), Thermodynamic equilibrium, Reprints, PROZPER computer program.

The authors have developed a predictive corresponding states model for the thermophysical properties of pure refrigerants and refrigerant mixtures. The bulk phase properties such as the density, enthalpy and entropy are predicted using the principle of extended cor-responding states. The theoretically based model uses shape factors to insure conformality among the vari-ous components and R134a is used as the reference fluid. The shape factors are found by mapping saturation boundaries of the fluids of interest onto the reference fluid. In the case where no saturation data are available, the shape factors are predicted. In addition to equilibrium properties, a one-fluid corresponding states model is used to predict the viscosity and ther-mal conductivity. Phase equilibria is predicted using a Peng-Robinson equation of state. The corresponding states model is contained in an interactive microcomputer program, PROZPER (PRoperties of OZone Protecting Environmentally acceptable Refrigerants). In addition, the program can 'learn' new components using only a minimum amount of information--the molecular weight, the normal boiling point and the critical parameters of the chemical species. Additional information such as vapor pressures, saturated liquid den-sities, saturated liquid thermal conductivities and vis-cosities may be input to improve the predictive capability of the model.

101,200

PB92-116946 Not available NTIS Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Building Equipment Div. Horizontal Flow Boiling Heat Transfer Experiments with a Mixture of R22/R114.

Final rept.

D. Jung, M. O. McLinden, R. Radermacher, and D. A. Didion. 1989, 15p Sponsored by Electric Power Research Inst., Palo

Alto, CA.
Pub. in International Jnl. of Heat and Mass Transfer 32, n1 p131-145 1989.

Keywords: \*Refrigerants, \*Thermodynamic properties, \*Heat transfer, \*Boiling, Heat transfer coefficient, Heat flux, Mixtures, Concentration(Composition), Liquid phases, Fluid flow, Transport properties, Reprints.

An experimental study on horizontal flow boiling heat transfer for pure R22 and R114 and their mixtures under uniform heat flux condition is reported. More than 1200 local heat transfer coefficients are obtained for annualar flow at a reduced pressure of 0.08 and

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qualities up to 85% for various heat fluxes and mass fluxes. The results show that local heat transfer coefficients for mixtures are as much as 44% lower than a linear mole fraction weighting of the pure component values for the same flow condition. A composition variation of up to 0.07 mole fraction in the annular liquid film was measured between the top and bottom of the tube. The effects of the composition variation and nonideal variations in physical properties account for the most of the heat transfer degradation seen with mix-

### Nonferrous Metals & Alloys

AD-A229 229/0 PC A10/MF A02 National Inst. of Standards and Technology, Boulder,

Aluminum Alloys for Cryogenic Tanks: Oxygen Compatibility. Volume 1.
Interim rept. Nov 88-Jun 90.
R. P. Reed, N. J. Simon, J. D. McColskey, and J. R. Berger. Sep 90, 207p AL-TR-90-063-VOL-1,

Keywords: Alloys, \*Aluminum alloys, Compatibility, Contamination, \*Cryogenics, Documents, Experimental data, Laboratories, \*Liquid oxygen, Oxygen, Portable equipment, \*Tanks(Containers), Test and evaluation, Test facilities, Test methods, \*Lithium alloys, \*Compatibility, Lox(liquid oxygen), Aluminum alloy 2090, Aluminum alloy 2219, Advanced Laupch System vanced Launch System.

In Part I of this program, Al-Li alloys 8090-T3 and 2090-T81 and Al alloy 2219 (tempers T851, T37) were tested for compatibility with liquid oxygen using pressurized mechanical-impact apparatuses at two NASA laboratories, Marshall Space Flight Center (MSFC) and White Sands Test Facility (WSTF). Specimens and data from tests at Santa Susana Field Laboratory (SSFL), Rocketdyne, on alloy 2090-T81 were supplied by ALCOA. Pressurized mechanical-impact data on alloy WL049-T351 were produced by WSTF. In addition, WSTF conducted open-cup mechanical-impact and promoted-combustion tests on all alloys. Reactions occurred in some specimens of all alloys during pressurized mechanical-impact tests at MSFC. There were no reactions during similar tests at WSFF and SSFL. The reactions at MSFC are not attributed to specimen contamination. This interim report analyzes the ignitions found in the MSFG pressurized mechanical impact tests compares the results and test methcal-impact tests, compares the results and test methodologies of both MSFC and WSTF facilities (since each laboratory is producing test data that are apparently divergent), and addresses the current test standard document NASA NHB 8060.1B as it pertains to this study. (TTL)

101,202 AD-A229 231/6 PC A09/MF A02 National Inst. of Standards and Technology, Boulder,

Review of Cryogenic Mechanical and Thermal Properties of Al-Li Alloys and Alloy 2219.

Final rpt. Nov 88-Jun 90.

N. J. Simon, E. S. Drexler, and R. P. Reed. Sep 90, 197p AL-TR-90-064,

Keywords: Air force facilities, Air force systems command, \*Aluminum alloys, Astronautics, Constants, \*Cryogenic storage devices, Cryogenics, Elastic prop-\*Cryogenic storage devices, Cryogenics, Elastic properties, Elongation, Fracture(Mechanics), High strength alloys, Laboratories, \*Launching, \*Lithium alloys, \*Mechanical properties, Specific heat, Supervisors, \*Tanks(Containers), Tensile strength, Thermal conductivity, Thermal expansion, \*Thermal properties, Toughness, Validation, Yield strength, Launchers, Alumibuth alloy 2219, Cryogenic tankage, Advanced Launch System.

The review of cryogenic mechanical and thermal properties presented here is part of a broader NIST program to assess new high-strength Al-Li alloys for use in the cryogenic tankage of the Advanced Launch System. This program is sponsored by the Air Force Systems Command, Astronautics Laboratory, Edwards Air Force Base, with Bao Nguyen, Task Manager. It is part of the Materials and Process Validation (3101) of the Structures, Materials, and Manufacturing (3000) portion of the ALS Advanced Development Pro-gram. Since the purpose of the NIST program has been to assess the relative suitability of high-strength Al-Li alloys and alloy 2219 for us in ALS cryogenic tanks, data on Al-Li alloys 8090, 2090, WeldaliteTM 049, and Al alloy 2219 have been included in the survey. Properties covered in this survey are tensile strength, yield strength, elongation, fracture toughness, elastic constants, specific heat, thermal conductivity, and thermal expansion. (ttl)

AD-A231 830/1 PC A07/MF A01 National Inst. of Standards and Technology, Boulder, CO.

Aluminum Alloys for ALS Cryogenic Tanks: Oxygen Compatibility. Volume 2. Final rept. Nov 88-Jun 90. R. P. Reed, N. J. Simon, J. D. McColskey, C. N. McCowan, and E. S. Drexler. Sep 90, 128p AL-TR-90-0630-VOL-2, See also Volume 1, AD-A229 229

Keywords: Alloys, Compatibility, Cryogenics, Drop tests, Electron microscopes, Electronic scanners, Eye, Gases, Height, Liquid oxygen, Lithium alloys, Magnifi-cation, Microscopy, Optical analysis, Oxygen, Potential energy, Power, Tanks(Combat vehicles), Test facili-ties. \*Aluminum alloys, Aluminum-lithium alloys, Weldalite.

In part II of this program, selected tempers of alloys 8090, 2090, WL049, and 2219 were tested for compatibility with liquid oxygen in modified open-cup and pres-surized mechanical-impact equipment at White Sands Test Facility. Drop height (potential energy), pressure, and environment (liquid oxygen, LOX, and gaseous oxygen, GOX were varied in these tests. Additional promoted-combustion tests were also conducted at WSTF. Reactions, ranging in size from those that could be observed with the naked eye to those that required use of the scanning electron microscope (SEM), were identified in all alloys. Those that require little or no magnifying power to view are labeled macroreactions; those that require the use of optical microscopy or SEM are called microreactions. Al-Li alloys had more macroreactions than 2219; 2219 had more, or an equivalent number of microreactions than each of the Al-Li alloys.

AD-A242 956/1 PC A07/MF A02 National Inst. of Standards and Technology, Boulder,

Aluminum Alloys for ALS Cryogenic Tanks: Comparative Measurements of Cryogenic Mechanical Properties of Al-Li Alloys and Alloy 2219. Final rept. Aug 89-Mar 90.

R. P. Reed, P. T. Purtscher, N. J. Simon, J. D.

McColskey, and R. P. Walsh. Oct 91, 146p

Keywords: \*Aluminum alloys, \*Lithium alloys, \*Cryogenics, Mechanical properties, Tensile properties, Fracture(Mechanics), Toughness, Delamination, Cracking(Fracturing), Low temperature alloys, Grain size, Aluminum - Lithium Alloys, Cryogenic Mechanical Properties, Alloy 2219, Surface Flaw.

Tensile and plane-strain fracture toughness properties were obtained at cryogenic temperatures to compare the AI-Li alloys 8090, 2090, and WL049 and alloy 2219 in various tempers and specimen orientations. The strongest alloy at very low temperatures is WL049-T851, which is about 10% stronger than 2090-T81. Both alloys are considerably stronger than 2219-T87. Alloy 2090-T81 is tougher in the in-plane orientations (about 50%) than WL049-T851 at low temperatures; the higher in-plane toughness is attributed to the pres-ence of less constituent particles and the tendency to crack out-of-plane or delaminate at low temperatures. This delamination tends to divide the moving crack, thus separating it into smaller regions where plan stress (rather than plane strain) conditions are conducive to increased toughness. Thus, a dichotomy: reduced toughness in the through-thickness or out-of-plane orientations leads to increased toughness in the in-plane orientations. In service, a leak in the tank is considered failure, and a leak will be caused by a crack in the panels of the tankage growing through the panel thickness. To measure the resistance to crack growth under these conditions, surface-flawed panel tests are recommended.

101.205 DE91016274 PC A03/MF A01 National Inst. of Standards and Technology, Boulder, Guideline for Nb(sub 3)Sn critical current measurements using fiberglass-epoxy composite sample mandrels.

L. F. Goodrich. 1989, 18p CONF-890701-31 Contract Al01-86ER52132

International cryogenic materials conference, Los Angeles, CA (United States), 24-28 Jul 1989. Sponsored by Department of Energy, Washington, DC.

Keywords: \*Critical Current, \*Niobium Base Alloys, Tin Alloys, Bonding, Composite Materials, Fiberglass, Intermetallic Compounds, Measuring Methods, Meetings, EDB/360104, \*Cryogenics, \*Superconductors.

This guideline was prompted, in part, by presentations given at the 6th Japan-US Workshop on High Field Superconductors (February 22--24, 1989, Boulder, CO) and subsequent discussions. The results of the recent Versailles Project on Advanced Materials and Stand-ards (VAMAS) Nb(sub 3)Sn critical-current round robin indicate that increased consistency in interlaboratory measurements might be achieved by a more detailed specification of the critical-current (l(sub c)) measurement technique. However, a competition exists be-tween the benefit of a rigidly specified measurement technique, which ensure measurement reproducibility, and a less restrictive technique that would be practical for a greater number of laboratories. Ideally, the measurement technique should have the least number of restrictions that is consistent with measurement repro-ducibility. This measurement guideline is intended to be one of a few different measurement techniques in a second Nb(sub 3)Sn I(sub c) round robin that is envisioned to determine the preferred measurement method for Nb(sub 3)Sn. At this time, there is no con-sensus regarding the materials used for the reaction mandrel, measurement mandrel, or sample bonding. There are advantages and disadvantages for all known materials. This guideline was written for one combination of materials. This measurement guideline assumes that the reader has the basic knowledge and experience with I(sub c) measurements of NbTi and Nb(sub 3)Sn conductors.

101,206

N91-21347/0

(Order as N91-21331/4, PC A24/MF A03) National Inst. of Standards and Technology (NML), Gaithersburg, MD. Thermophysics Div.

Dynamic Technique for Measuring Surface Tension at High Temperatures in Microgravity Environment.

A. P. Miiller, and A. Cezairliyan. 1 May 90, 5p In JPL, Proceedings of the First Workshop on Containerless Experimentation in Microgravity p 243-247.

Keywords: Heating, High temperature, \*Interfacial tension, \*Liquid metals, Melting, Microgravity applications, Pipes (Tubes), Reduced gravity, C-135 aircraft, Copper, Electric current, Melting points, Refractory metals, Simulation, Tantalum, \*Surface tension.

The feasibility of a dynamic technique for measuring surface tension of liquid metals at high temperatures in a microgravity environment was demonstrated. The basic method involves heating a tubular specimen resistively from ambient temperature through its melting point in about 1 sec by passing an electrical current pulse through it, while simultaneously recording the pertinent experimental quantities. Static equilibrium for the molten specimen is achieved in a microgravity environment by splitting the current after it passes through the specimen tube and returning a fraction along the tube axis, and the remaining fraction outside the specimen. Adjustments to the current split enable a balance between the magnetic and surface tension forces acting on the specimen. Values for surface ten-sion are determined from measurements of the equilibrium dimensions of the molten specimen tube, and the magnitudes of the currents. Rapid melting experiments, performed during microgravity simulations with the NASA KC-135 aircraft, yield a value for the surface tension of copper at its melting point which is in agree-ment with literature data. Measurements of surface tension of a refractory metal (tantalum) are underway.

101.207

PC A07/MF A01 PB91-132225 National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Metallurgy Div.

# Nonferrous Metals & Allovs

Institute for Materials Science and Engineering: Metallurgy Division, Technical Activities 1990. Annual rept. 1 Oct 89-30 Sep 90. E. N. Pugh, and J. H. Smith. Dec 90, 142p NISTIR-

See also report for 1989, PB90-161159.

Keywords: \*Metallurgy, Magnetic materials, Electrode-posited coatings, Corrosion, Processing, Process con-trol, Superconductors, Intermetallic compounds, High temperature tests, Heat resistant alloys, Steels, Microstructure, Weldments, Phase diagrams, Construction materials, Detectors, Metal matrix composites, International cooperation.

The report summarizes the FY 1990 activities of the Metallurgy Division of the National Institute of Standards and Technology (NIST). These activities center upon the structure-processing-properties relations of metals and alloys and on methods of measurement; and also include the generation and evaluation of criti-cal materials data. Efforts comprise studies of metals processing and process sensors; advanced materials, including metal matrix composites, intermetallic alloys and superconductors; corrosion and electrodeposi-tion; mechanical properties; magnetic materials; and high temperature reactions. The work described also includes two cooperative programs with professional societies (the Alloy Phase Diagram Program with ASM International, and the Corrosion Data Program with the National Association of Corrosion Engineers); two with trade associations (the Temperature Sensor Program with the Aluminum Association, and the Steel Sensor Program with the American Iron and Steel Institute); and several with industry including the Powder Atomization Consortium with three companies.

101.208 Not available NTIS PB91-134551 National Bureau of Standards (IMSE), Gaithersburg, MD. Metallurgy Div.

Literature Review of the Galling Process.

Final rept.

M. B. Peterson, L. K. Ives, and K. J. Bhansali. 1987,

Pub. in Proceedings of Symposium on Metal Transfer and Galling in Metallic Systems, Orlando, FL., October 8-9, 1986, p1-25 1987.

Keywords: \*Galling, \*Reviews, \*Metals, Plastic deformation, Surface roughness, Microstructure, Crystal structure, Loads(Forces), Strain hardening, Reprints, Preferred orientation, Temperature dependence, Asperity.

A review was conducted of the technical literature relating to the process of galling. Approximately 250 references pertinent to galling were reviewed and key ref-erences selected. A principal focus of the review concerned the relationship between galling and plastic deformation. Attention was directed to two deformation models; a soft asperity model and a hard asperity model. From these models a postulate on frictional behavior has been developed. The severity of galling is determined not only by contact conditions such as load and contact geometry but also by factors affecting deformation characteristics such as crystal structure, preferred orientation, work hardening rate, and microstructure. The severity of galling is found to increase with increasing load, reduced surface roughness, higher adhesion, reduced strain hardening rate and higher temperature. These and other factors relating to galling severity are discussed.

101.209 PB91-147314 Not available NTIS National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Metallurgy Div. Phase Formation in Electrodeposited and Thermally Annealed Al-Mn Alloys. Final rept.

B. Grushko, and G. R. Stafford. 1990, 11p Sponsored by Office of Naval Research, Arlington, VA. Pub. in Metallurgical Transactions A 21A, p2869-2879 Nov 90.

Keywords: \*Aluminum manganese alloys, Amorphous materials, Electrodeposition, Aluminum intermetallics, Annealing, Icosahedrons, BCC lattices, FCC lattices, Reprints, Icosahedral phase, Quasicrystals, Manganese intermetallics.

Aluminum-manganese alloys with compositions ranging from 0 to 50 wt pct Mn were electrodeposited onto copper substrates from a chloroaluminate molten salt electrolyte containing MnCl2 at temperatures of 150 C

to 325 C. The structures of these electrodeposits were then compared to those observed when metastable electrodeposits were thermally annealed at 200 C to 610 C. The alloys were characterized by scanning electron microscopy, transmission electron microscopy (TEM), energy dispersive spectroscopy, and X-ray diffraction. At deposition temperatures of 150 C to 250 C, no stable structure other than the strongly supersaturated and highly dislocated Al-face-centered cubic (fcc) solid solution is observed. An amorphous phase and body-centered cubic (bcc) Al8Mn5 are observed at higher manganese compositions.

101,210 PB91-147322 PB91-147322 Not available NTIS National Bureau of Standards (IMSE), Gaithersburg, MD. Metallurgy Div.
Effect of Coherency Strain on Alloy Formation: Mi-

gration of Liquid Films. Final rept.

C. A. Handwerker, J. W. Cahn, D. N. Yoon, and J. E. Blendell. 1985, 18p Sponsored by Army Research Office, Research Trian-

gle Park, NC. Pub. in Proceedings of TMS-AIME Fall Meeting Diffusion in Solids: Recent Developments, Detroit, Ml., September 17, 1984, p275-292 1985.

Keywords: \*Alloys, Mathematical models, Thermodynamics, Diffusion, Reprints, \*Liquid films.

When solid solution grains are not in chemical equilibrium with the liquid in which they are imbedded, equilibration frequently occurs by dissolution and reprecipitation of saturated solid solution, rather than by solid state diffusion. At small volume fractions of liquid, this mechanism has the appearance of liquid film migration and is modelled by diffusion of the components of the solid through the liquid film, driven by differences in solubility in the liquid between the dissolving grain and the growing grain. A thermodynamic analysis is given for the solubilities of the grains, which includes local interfacial curvature and local coherency stresses due to lattice parameter variations in the diffusion zones. An expression for the migration velocity derived from the model contains no unmeasurable parameters. Except for curvature and liquid film thickness, the parameters are all thermodynamic, elastic, crystallographic or diffusive and can be measured independent of the liquid film migration process.

101,211 PB91-147512 Not available NTIS National Bureau of Standards (IMSE), Gaithersburg, MD.

Phase Diagrams of Hexagonal Binary Ordering Alloys with Anisotropic Interactions. Final rept.

R. Kikuchi, and J. W. Cahn. 1987, 6p Pub. in Proceedings of International Conference on User Applications of Alloy Phase Diagrams, Lake Buena Vista, FL., October 4-9, 1986, p19-24 1987.

Keywords: \*Binary alloys, \*Phase diagrams, Hexagonal close packed lattices, Order disorder transformations, Interactions, Reprints, Cluster variation method.

Phase diagrams between the disordered and the DO(19) ordered (A(3)B) phases are calculated for the hexagonal lattice using the tetrahedron approximation of the cluster-variation method. Nearest-neighbor pairwise interactions are assumed, but the bonds within the basal plane are allowed to differ from the bonds between basal planes, r being the ratio of interaction energies. When r = 1, the disorder-A(3)B phase boundary agrees exactly with that calculated for fcc, although the entropy expressions for the hcp and fcc cases are different. For 0.8 < r < 1.2, the boundary shape is qualitatively the same as the r=1 case. When 0 < r < 0.7, the present calculations for the Brich side of the A(3)B phase becomes unstable.

PB91-147637 Not available NTIS National Bureau of Standards (IMSE), Gaithersburg, MD. Ceramics Div. Structure of Surface Films on Magnesium and on Magnesium Alloys. Final rept.

G. G. Long, J. Kruger, D. K. Tanaka, and Z. Zhang. 1988, 1p Pub. in Jnl. of the Electrochemical Society 135, n3

pC144 1988.

Keywords: \*Magnesium oxides, \*Magnesium, \*Surfaces, X ray spectroscopy, Crystal structure, Oxygen, Films, Reprints, \*Magnesium alloy AZ61. Surface reflection x-ray spectroscopy measurements at the oxygen K-edge are reported for surface films on high purity magnesium and on AZ61 magnesium alloy. Surface-EXAFS data was extracted for the films and for a single crystal MgO standard sample. The experimental curves were fitted by theoretical curves to obtain oxygen nearest neighbor distances, coordination numbers, and a measure of the disorder in the sur-

PB91-148866 Not available NTIS National Bureau of Standards (IMSE), Gaithersburg,

MD. Reactor Radiation Div.

Neutron Powder Diffraction and Inelastic Scattering Study of the Structures of Zr2Pd, Zr2PdD1.70, and Zr2PdD1.96.

Final rept.

A. J. Maeland, E. Lukacevic, J. J. Rush, and A. Santoro. 1987, 15p Pub. in Jnl. of the Less Common Metals 129, p77-91

Feb 87.

Keywords: \*Zirconium hydrides, \*Palladium, \*Alloys,

Crystal structure, Deuteration, Isotope effects, Neutron diffraction, Intermetallic compounds, Tetragonal lattices, Reprints.

The compounds Zr2Pd, Zr2PdD 1.70, and Zr2PdD 1.96 have been studied with the neutron powder diffraction technique and the Rietveld method of profile analysis. All three materials crystallize with the symarraysis. All thee materials crystalize with the symmetry of space group I4/mmm, Z=2. The lattice parameters are a = 3.3085(9) and c = 10.8907(6) lambda for Zr2PdD 1.70, and a = 3.3715(3) and c = 11.438(2) lambda for Zr2PdD 1.96. The D atoms are located at the centers of slightly distorted tetrahedra of Zr atoms with a Zr-D distance of 2.071(1) lambda in Zr2PdD 1.70 and 2.092(2) in Zr2PdD 1.96 and with Zr-D-Zr angles ranging from 106.6 deg to 110.9 deg. The hydrogen location in the structure has been confirmed by neutron inelastic scattering measurements. These show a broad hydrogen vibration peak at 135 meV analogous to that observed for hydrogen bound in relatively undistorted tetrahedral sites in other hydrides. As a consequence of the insertion of deuterium in the structure of the intermetallic compound, the Zr-Zr distances in the deuterides are considerably different from the corresponding ones intermetallic compound, the Zr-Zr distances in the deuterides are considerably different from the corresponding ones in Zr2Pd. However the Zr-Pd separation remains practically identical in the three materials.

101,214

PB91-149039 Not available NTIS National Bureau of Standards (IMSE), Gaithersburg, MD. Metallurgy Div.

Materials Research at the National Bureau of Standards.

Final rept.

E. N. Pugh. 1986, 3p Pub. in Proceedings of Materials Technology Congress, Adelaide, Australia, May 19-21, 1986, v1 p1-3.

Keywords: \*Research projects, \*Metals, \*Nondestructive tests, \*US NBS, International cooperation, Australia, Processing, Reprints.

Materials research at NBS is centered in the Institute for Materials Science and Engineering, one of four major organizational units at the Bureau. The Institute is comprised of five Divisions, namely Ceramics, Fracture and Deformation, Metallurgy, Polymers, and Reactor Radiation; it also manages a Bureau wide interdisciplinary program in nondestructive evaluation. As an agency of the Department of Commerce, NBS has traditionally provided the measurement foundation to support our industrial economy, and the Institute continues to generate measurement methods, critical materials data and standards for the industrial and scientific community. The Institute's research programs support the measurement activities and, in addition, are moving increasingly to address the science base underlying both traditional and new materials technologies. The lecture outlines these activities, focusing mainly on those of the Metallurgy Division and the NDE program.

101,215

PB91-149427 Not available NTIS National Inst. of Standards and Technology (IMSE), Gaithersburg, MD. Polymers Div.

# Nonferrous Metals & Alloys

Structural Instabilities and Superconductivity in Quasi-Binary Mn5Si3-Type Compounds. Final rept.

R. M. Waterstrat, R. Kuentzler, and J. Muller. 1990, 10p

Sponsored by American Dental Association Health Foundation, Chicago, IL.

Pub. in Jnl. of the Less-Common Metals 167, p169-178 1990.

Keywords: \*Binary alloy systems, \*Superconductivity, \*Zirconium alloys, \*Platinum alloys, Iridium alloys, Osmium alloys, Specific heat, Magnetic permeability, Gold additions, Transition temperature, Low temperature, Reprints, Manganese silicides.

Measurements have been made of the low temperature specific heat, magnetic susceptibility, lattice parameters and superconducting behavior of quasi-binary compounds based on the Mn5Si3-type structure and having the general formula Zr5lr(1-v)Tv where T is either platinum or osmium. The atomic displacements previously reported for the Zr5lr3 structure occur only near this binary composition: other alloys in the quasi-binary systems have an undistorted Mn5Si3 type structure. Superconductivity occurs in these quasi-binary systems, and Tc is a continuous function of the electron concentration reaching a maximum of Tc = 7.2 K for the binary compound Zr5Pt3. Substitution of small amounts of gold for platinum in Zr5Pt3 apparently destabilizes the Mn5Si3 type structure and produces alloys of unknown structure with lower Tc values (about 4 K).

101,216 PB91-149450 Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Automated Production Technology Div. Material Dependency of Chip-Form Detection Using Acoustic Emission.

Final rept. K. W. Yee. 1987, 5p

Pub. in Proceedings of NAMRC (North American Manufacturing Research) Conference (15th), Bethlehem, PA., May 27-29, 1987, p458-462.

Keywords: \*Chips, \*Machining, \*Acoustic detectors, \*Metal spinning, Microcomputers, Monitoring, Aluminum, Steels, Metal products, Metal scrap, Metal working, Reprints.

An acoustic-emission-based microcomputer chip-form monitor has been designed and built at the National Bureau of Standards. The monitor implements algorithms based on research by the University of California, Berkeley. The ability to identify chip form in turning of three types of metal (aluminum, low-carbon steel, and an alloy steel) has been previously reported. The monitor performs best for the easy-to-machine metals where chip breaking is most difficult and disastrous tangles are most likely. Subsequent experiments have shown that the successful identification of chip form is dependent on the work-place metal. Additional results from the machining of two-nonmagnetic stainless steels and a copper alloy are contrasted with the previous results.

PB91-158485 Not available NTIS National Inst. of Standards and Technology (MSEL),

Gaithersburg, MD. Reactor Radiation Div.
Rapid Low-Temperature Hopping of Hydrogen in a
Pure Metal: The ScHx System.

Final rept. I. S. Anderson, N. F. Berk, J. J. Rush, T. J. Udovic, R. G. Barnes, A. Magerl, and D. Richter. 1990, 4p. Pub. in Physical Review Letters 65, n12 p1439-1442, 17 Sep 90.

Keywords: \*Scandium, \*Hydrogen, Low temperature research, Neutron scattering, Structure factors, Diffusion, Reprints.

The localized motion of hydrogen in scandium has been studied by quasielastic neutron scattering. The results reveal that the quasielastic linewidth has a pronounced minimum near 100 K and rises at lower temperature with approximate 1/T dependence, indicative of nonadiabatic behavior that can be associated with weak coupling of hydrogen to the metal conduction electrons. This is the first such observation in a pure-metal-hydrogen system. The simultaneous determination of the elastic incoherent structure factor is interpreted in terms of labile and nonlabile hydrogen configurations in a manner consistent with recent estimates of pairing and activation energies in the rare-earth-hydrogen systems.

101,218 PB91-158527 Not available NTIS National Bureau of Standards (IMSE), Gaithersburg, MD. Metallurgy Div.

Acoustic Emission Monitoring of Laser Drilling. R. B. Clough, R. J. Schaefer, and H. N. G. Wadley.

1984, 10p Pub. in Proceedings of ASM Metals Congress Metals/

Materials Technology Series, Detroit, Ml., September 15-10, 1984, p1-10.

Keywords: \*Metals, \*Laser drilling, \*Acoustic emission, Manufacturing, Nondestructive tests, Process control, Laser radiation, Aluminum, Reprints.

Laser drilling, because of its speed, controllability, and ability to penetrate tough or exceptionally hard materials, is a rapidly growing manufacturing method. However, beam power spikes and interventing disintegration products can disrupt or diminish energy transmis-sion to the hole site, resulting in variable hole depth. To improve the situation, a combination of acoustic emission monitoring and laser settings has been investigated to improve hole depth prediction. The emission suggested to be generated principally by liquid expulsion; intergranular cracking appears to be a secondary source. Acoustic emission shows promise as an experimental method for study of directed energy beam-material interactions.

101,219 PB91-158550 Not available NTIS National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Metallurgy Div. Convective and Morphological Instabilities during

Directional Solidification.

Final rept. S. R. Coriell, and G. B. McFadden. 1990, 15p Sponsored by National Aeronautics and Space Administration, Washington, DC.

Pub. in Principles of Solidification and Materials Processing, Chapter 16, v1 p365-379 1990.

Keywords: \*Directional solidification(Crystals), \*Binary alloys, Liquid-solid interfaces, Convection, Rayleigh scattering, Crystal growth, Separation, Morphology, Finite difference theory, Liquid metals, Stability, Mathematical models, Time dependence, Reprints.

During the directional solidification of a binary alloy at During the directional solidification of a binary alloy at constant velocity, solute segregation may arise due to either interface instability or fluid flow in the melt. Recent calculations of cellular shapes in the absence of fluid flow and thermosolutal convection caused by the rejection of a lighter solute during growth vertically upwards are presented. Three-dimensional steadystate solutions for nonplanar interface morphologies are computed numerically by finite differences. A linear temperature field is assumed, and the solute field in the melt and the unknown crystal-melt interface position are obtained self-consistently. For a model of an alumimun-chromium alloy with a distribution coefficient greater than unity, the calculations predict hexagonal nodes near the onset of instability. Numerical results for the solute segreation caused by thermosolutal convection are obtained using finite differences in a twodimensional, time-dependent model that assumes a planar-crystal melt interface. The system is assumed periodic in the horizontal direction, and the possibility of multiple flow states sharing the same period is examined. As the solutal Rayleigh number is varied, multiple steady states, time-periodic states, and quasiperiodic states occur.

PB91-158949 Not available NTIS National Bureau of Standards (IMSE), Gaithersburg, MD. Metallurgy Div. Rapid Solidification Alloys: Crystals, Quasicrys-

tals, and Metallic Glass. Final rept.

J. R. Manning, 1986, 6p

Pub. in ASTM (American Society for Testing and Materials) Standardization News 14, n9 p26-31 Oct 86.

Keywords: \*Metals, \*Alloys, Reviews, Phase tranformations, Metallic glasses, Microstructure, Reprints, \*Quasicrystals, \*Rapid solidification process.

An overview is given of rapid solidification processes and the advantages rapid solidification can provide to alloys. The advantages include finer microstructures, decreased segregation, extended solid solubility, and formation of new types of phases, including the recently discovered quasicrystal phases.

101.221

PB91-158964 Not available NTIS National Bureau of Standards (IMSE), Gaithersburg,

MD. Metallurgy Div.
Transformation of the Icosahedral Phase in Rapidly Quenched Al-rich Al-Mn Alloys.

**Final** rept

A. J. McAlister, L. A. Bendersky, R. J. Schaefer, and F. S. Biancaniello. 1987, 4p Pub. in Scripta Metallurgica 21, n2 p103-106 1987.

Keywords: \*Aluminum manganese alloys, Phase ransformations, Crystallization, Icosahedrons, Aluminum intermetallics, Thermal analysis, X ray diffraction, Electron microscopy, Activation energy, Reaction kinetics, Heat of crystallization, Reprints, "Quasicrystals Leachorful phage Management intermetallics" tals, Icosahedral phase, Manganese intermetallics.

Crystallization of the quasicrystalline icosahedral phase formed in Al-rich Al-Mn alloys has been studied by constant heat rate DTA, XRD, and TEM. Heats and activation energies of transformation were obtained. and evidence presented which suggests that the transformation is diffusion controlled.

101.222

PB91-159111 Not available NTIS National Bureau of Standards (IMSE), Boulder, CO. Fracture and Deformation Div.

Use of Neutron Pole Figures to Calibrate Ultrasonic Techniques for On-Line Texture Control of Aluminum Plates.

Final rept.

Final rept.

R. C. Reno, A. V. Clark, G. V. Blessing, R. J. Fields, A. Govada, R. B. Thompson, P. P. Del Santo, R. B. Mignogna, and J. F. Smith. 1987, 7p

Pub. in Proceedings of ASM Symposium on Intelligent Processing of Materials and Advanced Sensors, Or-

lando, FL., 1986, p77-83 1987.

Keywords: \*Metal plates, \*Aluminum, \*Neutron diffraction, \*Process control, Intelligence, Calibrating, Ultrasonic tests, Texture, Metal rolling, Crystallography, On-line systems, Monitors, Detectors, Comparison, Nondestructive tests, Reprints.

Neutron pole figures were used to determine the crystallographic texture in rolled aluminum plates that were previously characterized with ultrasonic techniques. The orientation distribution function coefficients (ODC's) determined by neutron diffraction are in excellent agreement with those derived from ultrasound measurements, thus confirming the efficacy of ultrasound as an on-line monitoring technique.

PB91-159202 Not available NTIS National Bureau of Standards (IMSE), Gaithersburg, MD. Metallurgy Div. Electrodeposition of Aluminum from Molten Salts.

G. Stafford, and C. Turner. 1987, 13p Pub. in AESF Annual Technical Conference, v74 13p 1987

Keywords: \*Electrodeposition, \*Aluminum manganese alloys, \*Fused salts, Amorphous materials, Aluminum intermetallics, Electrolytes, Manganese additions, Metallic glasses, Heat treatment, X ray diffraction, Reprints, Manganese intermetallics.

The effect of additions of Mn to molten salt electrolytes will be discussed. It was found that aluminum manganese alloys exhibit x-ray diffraction patterns consistent with a metallic glass structure which upon heat treatment transforms to the crystalline intermetallic Al6Mn. Some electrochemical phenomena operative in these melts will be discussed.

101.224

PB91-167338 PC A04/MF A01 National Inst. of Standards and Technology, Gaithersburg, MD. Intercomparison Study of Rockwell Hardness Test

Blocks. T. R. Shives, and J. H. Smith. Feb 91, 74p NISTIR-4531

Keywords: \*Standards, \*Rockwell hardness, \*Metals, Comparison, Test equipment, Diamond pyramid hardness tests, Aging tests (Materials), Calibrating.

The National Institute of Standards and Technology undertook an intercomparison study of Rockwell hard-

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ness test blocks marketed in the United States. Test blocks from six different manufacturers were included in the study. Measurements were made generally on seven sets of test blocks at three hardness levels for each of the HRC, HRB, HR30N and HR30T hardness scales. Even for the nearly ideal conditions of the study, it was found that there are significant differences among hardness test blocks of different manufacturers for some hardness levels. This is especially true for the high hardness part of the HRC scale, the lower and middle parts of the HRB scale, and parts of both the HR30N and HR30T scales. In these regions, the ranges of test results for blocks of different manufacturers. facturers that have similar assigned values exceed the tolerance limits for standardized test blocks according to ASTM Standard E 18-89a. Reevaluation of HRB and HR30T test blocks four to five years after initial evaluation indicated that many of these are unstable. There were significant changes in hardness in a number of the blocks.

101,225 PB91-174466 PB91-174466 Not available NTIS National Bureau of Standards (IMSE), Gaithersburg, MD. Reactor Radiation Div.

Properties of Amorphous Zirconlum Rhodium Hydride (Zr3RhHx) Prepared from Glassy and Crystalline Alloys.

talline Alloys.
Final rept.
R. C. Bowman, J. S. Cantrell, K. Samwer, J. Tebbe,
E. L. Venturini, and J. J. Rush. 1988, 13p
Pub. in Physics Review B: Condensed Matter 37, n15

Keywords: \*Amorphous materials, \*Zirconium alloys, \*Rhodium alloys, \*Metal hydrides, Metallic glasses, Hydrogenation, Neutron scattering, Nuclear magnetic resonance, Electronic structure, Thermal degradation, Magnetic permeability, X ray diffraction, Calorimetry, Reprints.

The a-Zr3RhHx samples with x < 5.5 were studied by x-ray diffraction, proton nuclear magnetic resonance, magnetic susceptibility, low temperature heat capacity, differential scanning calorimetry, and inelastic neutron scattering. All hydride samples are amorphous with similar properties which are shown to be independent of the structure for the initial alloy. Namely, the solid-state reaction of hydrogen with crystalline c-Zr3Rh appeared to produce an equivalent amorphous phase to hydrogenated glassy alloys. The changes in the electronic and magnetic properties upon hydrogenation imply a systematic decrease in the Fermi level density of states in a-Zr3RhHx as the hydrogen content increases. The thermal stabilities of the amorphous hydrides (with respective to the irreversible formation of crystalline ZrHx phases) also decrease with increasing hydrogen stoichiometry. Whereas the hydrogen atoms predominantly occupy tetrahedral interstitial sites coordinated with zirconium atoms there is strong circumstantial evidence for occupancies of different and less stable sites at the higher compositions.

PB91-174771 Not available NTIS National Bureau of Standards (IMSE), Gaithersburg,

N-Dimensional Crystallographic Description of the Icosahedral Phases; the Example of the AI73Mn21Si6 Quasiperiodic Structure. Final rept.

D. Gratias, J. W. Cahn, M. Bessiere, Y. Calvayrac, S. Lefebvre, A. Quivy, and B. Mozer. 1987, 12p Pub. in Proceedings of NATO Advanced Research Workshop, Italy, October 4-8, 1987, 12p.

Keywords: \*Aluminum alloys, \*Icosahedrons, \*Phase diagrams, X ray diffraction, Neutron diffraction, Electron diffraction, Crystallography, Reprints, Quasiperio-

Icosahedral phases in aluminium based alloys have been extensively studied by means of x-ray, neutron and electron diffraction. Many spectra have been collected, but no fully satisfying crystallographic model that matches properly the observed diffracted intensi-ties has been proposed. The structural characterization of quasiperiodic phases is a formidable task due to the numerous parameters which have to be determined in addition to those of standard 3D crystallography.

101,22/ PB91-187161 Not available NTIS National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Metallurgy Div.

Role of Elastic Energy in the Morphological Development of a Ni-Ti-Al Alloy. Final rept.

L. A. Bendersky, P. W. Voorhees, W. J. Boettinger,

and W. C. Johnson. 1988, 6p Pub. in Scripta Metallurgica 22, n7 p1029-1034 Jul 88.

Keywords: \*Strain energy methods, \*Morphology, \*Nickel alloys, \*Titanium alloys, \*Aluminum alloys, Clastic Cooling, Flantin alloys, Audinin alloys, Flastic Microstructure, Quenching(Cooling), Electron microscopy, Annealing, Phase transformations(Materials), Transmission electron microscopy, Heusler alloys, Precipitates, Coherence, Reprints, \*Rapid solidification process.

The late-stage microstructural development of a rapidly solidified Ni50Ti37.5 alloy, studied by TEM is described. During 800 C annealing, the following transformations occur: Heusler single phase to modulated precipitation of B2 phase to cuboidal precipitates of Heusler phase in B2 matrix to interconnected Heusler/ B2 structure. The morphological evolution of the co-herent system is controlled primarily by elastic strain

101,228 PB91-187187 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Building Materials Div.

Characterization of Cylindrical Holes in Metallic

Substrates via Their Infrared Emission Patterns. Final rept.

D. P. Bentz, J. W. Martin, and M. E. Batts. 1991, 12p Pub. in Wear 143, p255-266 1991.

Keywords: \*Thermal emission, \*Holes(Mechanics), \*Aluminum, \*Steels, \*Metals, \*Infrared mapping, Infrared thermal detectors, Metal plates, Depth measurement, Temperature measuring instruments, Comparison, Theories, Milling(Machining), Geometry, Substrates, Ambient temperature, Calibrating, Surface energy, Reprints.

IR emission patterns for a series of cylindrical holes milled into aluminum and steel plates were compared with those predicted from existing theory. The emis-sion patterns were found to be influenced by the hole geometry, the substrate material and the IR camera geofficing, the substitute final fin steel plate, however, the theory was found not to apply and empirical calibration was required. It is concluded that the IR technique may have promise in characterizing the diameter and depth of milled holes at temperatures near ambient.

101 229 PB91-187203 Not available NTIS National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Metallurgy Div. Particle Size Measurement of Inert Gas Atomized

Final rept.
F. S. Biancaniello, J. J. Conway, P. I. Espina, G. E. Mattingly, and S. D. Ridder. 1990, 6p
Pub. in Materials Science and Engineering A A124, n1

p9-14, 10 Apr 90. Keywords: \*Atomizers, \*Powder metallurgy, \*Particle size distribution, \*Supersonic flow, Measurement, Metal powder, Reliability, Reproducibility, Graphic methods, Reprints, \*Supersonic inert gas metal atom-

Metal powder produced by a Supersonic Inert Gas Metal Atomizer (SiGMA) has been analyzed by using several diagnostic methods. These analyses have brought several interesting results. Some of these un-expected results are the reliability of the various tech-niques, the procedures for proper (reproducible) particle size analysis, and the graphical representation of the data that best shows the powder characteristics. The study has shown that gas atomized powder produced in the SiGMA facility has distinct size distribution characteristics that do not follow the log-normal pat-tern. The fragmentation mechanisms leading to droplet formation are examined which explain the SiGMA powder size distribution data. These powder analysis procedures are applicable to all inert gas atomized powder and could lead to a better understanding of the atomizing system's operative liquid disruption mecha-

101,230 PB91-187252

Not available NTIS

National Inst. of Standards and Technology (IMSE), Gaithersburg, MD. Reactor Radiation Div.

Relationship of Hydrogen Site Occupancy to Diffusion Behavior in Crystalline and Amorphous

Final rept. R. C. Bowman, D. R. Torgeson, R. G. Barnes, A. J. Maeland, and J. J. Rush. 1989, 6p Pub. in Z. Phys. Chem. 163, n2 p425-430 1989.

Keywords: \*Amorphous materials, \*Zirconium alloys, \*Palladium alloys, \*Zirconium hydrides, \*Diffusion, Neutron scattering, Neutron diffraction, Nuclear magnetic resonance, Relaxation time, Crystal structure, Surface chemistry, Protons, Reprints.

New measurements of the proton relaxation times have resulted in more thorough analyses of the diffusion properties in crystalline and amorphous Zr2PdHx. The influences of host metal and hydrogen site occupancies were better recognized when additional information from the proton second moments, inelastic neutron scattering spectra, and published neutron dif-fraction data was included. Complex motion is indicated when multiple sites become occupied at the higher stoichiometries of the crystalline phases or in the glassy hydride.

101.231

PB91-189423 Not available NTIS National Inst. of Standards and Technology (IMSE), Gaithersburg, MD. Metallurgy Div. Structural Study of Electrodeposited Aluminum-

Manganese Alloys. Final rept.

B. Grushko, and G. Stafford. 1989, 9p Pub. in Metallurgical Transactions A 20, n8 p1351-1359 1989.

Keywords: \*Aluminum alloys, \*Manganese additions, Reywords: "Aluminum alloys, "Manganese additions, "Electrodeposited coatings, Phase transformations(Materials), Liquid metals, Compositions, FCC lattices, Substrates, Copper, Amorphous materials, Binary alloys, X-ray diffraction, Electron microscopy, Aluminum chlorides, Solutes, Reprints, "Rapid solidification process, Icosahedral phase.

Al-Mn alloys with compositions ranging between 0-27 wt% Mn were electrodeposited at 150C onto copper substrates from a chloroaluminate melt with controlled addition of MnCl2. The specimens were studied by SEM, TEM, EDAX and x-ray diffraction. The addition of small amounts of Mn results in the formation of a supersaturated fcc solid solution of Mn in Al. At the higher Mn content an amorphous phase is established. The highly facted crystalline surface of pure Al and Al-Mn solid solution becomes a smooth nearly specular surface when the amorphous phase is present. There is a concentration discontinuity between the above limit and the higher Mn concentration limit of the fcc phase (about 9 wt%). Appearance of the amorphous phase in the alloy results in a decrease in the Mn concentration in solid solution to about 2 wt%. The crystallization of the amorphous phase starts at the fcc-amorphous phase interface at 230C. As a result of treatment at 230-340C, the amorphous phase completely transforms into Al6Mn, while the fcc phase is unaffected. Prior to crystallization, the amorphous phase shows a modification that could be interpreted as the formation of fine-grain icosahedral phase. The forma-tion of phases by electrodeposition and rapid solidification is discussed.

PB91-189696 Not available NTIS National Inst. of Standards and Technology (IMSE), Gaithersburg, MD. Metallurgy Div. Surface Properties and Coatings of Materials Mi-

crotailored Alloys. Final rept.

D. Lashmore. 1988, 7p Pub. in Israel Jnl. of Technology 24, n3-4 p469-475 1988

Keywords: \*Electrochemical coating, \*Electrodeposition, \*Process control, \*Alloys, Compositions, Surface properties, Microstructure, X-ray diffraction, Copper alloys, Cobalt alloys, Nickel alloys, Interfaces, Reprints.

Electrochemical deposition is becoming recognized as an important processing technique to produce alloys whose properties can be controlled on a near atomic level. In the paper alloy deposition is reviewed with particular emphasis on a deposition process incorpo-

# Nonferrous Metals & Allovs

rating a feedback system allowing a high degree of control over composition. Such a process can be used to produce unique microstructures which may be tailored on a near atomic level resulting in materials whose properties may be very finely tailored. Such a control has implication for the design of new alloys whose interfacial properties must be precisely con-

PB91-189985 Not available NTIS National Inst. of Standards and Technology (MSEL), Boulder, CO. Fracture and Deformation Div. PB91-189985

Creep of Copper: 4 to 295 K.

Final rept. R. P. Reed, N. J. Simon, and R. P. Walsh. 1990, 9p. Sponsored by Department of Energy, Washington, DC. Pub. in Advances in Cryogenic Engineering, v36 p1175-1183 1990.

Keywords: \*Copper, \*Creep properties, \*Creep tests, Least squares method, Strains, Shear properties, Tensile properties, Steady state, Mechanical properties, Shear flow, Experimental data, Reprints.

Creep measurements at 295, 76 and 4 K have been conducted on C10400 copper. Specimens were held under constant tensile load (dead weight) for periods of time sometimes exceeding one month. Creep data have been fitted to a series of expressions relating creep strain to time by a nonlinear least-squares procedure. The coefficients of the terms in the equations were related to applied stress levels. Primary, logarithmic, and steady-state creep ranges are discussed.

101,234 PB91-194852 Not available NTIS National Inst. of Standards and Technology (MSEL), Boulder, CO. Fracture and Deformation Div. Elastic Constants of a Tungsten-Particle Copper-Matrix Composite.

Final rept. H. Ledbetter, and S. Datta. 1991, 4p Pub. in JSME International Jnl., Series I, v34 n2 p194-

Keywords: \*Elastic properties, \*Metal matrix composites, \*Particulate composites, \*Copper, \*Tungsten, Ultrasonic tests, Young modulus, Shear strength, Bulk modulus, Mathematical models, Poisson ratio, Anisotropy, Reprints.

Using a megahertz-frequency ultrasonic method, a measurement of the elastic constants of a composite consisting of seventy-volume-percent tungsten particles in a copper matrix was done. The Young, shear, and bulk moduli and the Poisson ratio are reported. and bulk moduli and the Poisson ratio are reported. Tungsten is much stiffer than copper: the Young-mod-ulus ratio equals 410/129=3.2. Thus, from a linear rule-of-mixture, large departures were found. (The Poisson ratio comes close to a linear rule-of-mixture.) Unexpectedly, a substantial elastic anisotropy was found: eighteen percent in the shear modulus. To model the system, a scattered-plane-wave ensemble-average approach was used. For the four elastic constants listed above, reasonable model-measurement agreement was found, one-to-seven percent for the averaged-over-direction measurements. Assuming oblatespheriodal (c/a = 0.5) particles improves the agreement: two percent or less for the four cases.

PB91-195537 Not available NTIS National Bureau of Standards (IMSE), Gaithersburg,

MD. Metallurgy Div.

Coherency Strain Induced Instability of Solid-Liquid Interfaces in the Mo-NI System.

Final rept. W. H. Rhee, C. A. Handwerker, and D. N. Yoon.

1988, 7p Pub. in Proceedings of MRS Symposium on Interfacial Structure, Properties and Design, v122 p205-211

Keywords: \*Instability, \*Liquid-solid interfaces, \*Molybdenum alloys, \*Nickel alloys, \*Binary alloys, Time dependence, Equations, Microstructure, Diffusion Grain boundaries, Migration length, Films, Grain growth, Liquid metals, Liquids, Reprints, Coherency

An instability at solid-liquid interfaces induced by coherency strain has been studied in the Mo-Ni system. The coherency strain is developed in the diffusion zone by solute diffusion into the solid when the lattice parameter varies with composition. As a result of the

strain, the originally planar solid-liquid interface be-comes unstable by dissolution of the initial solid and reprecipitation of the new solid, forming a sinusoidal interface shape. In a previous study, the coherency strains have been shown to be the driving force for the strains have been shown to be the driving loce for the solution and reprecipitation process of the instability. The paper analyzes the evolution of the instability with time, from initiation to healing of the instability. Using the equations developed for liquid film migration (LFM) the change of microstructure is explained qualitatively. In addition, the relationships between the instability and diffusion induced grain boundary migration (DIGM) and LFM are discussed.

101,236 PB91-195651 Not available NTIS National Inst. of Standards and Technology (IMSE), Gaithersburg, MD. Metallurgy Div. Phase Selection in Non-Equilibrium Processing.

Pillar Tept.

R. J. Schaefer. 1989, 14p

Pub. in Proceedings of Indo-US Workshops on Solidification Principles and Materials Processing, Hyderabad, India, January 15-21, 1988, p381-394 1989.

Keywords: \*Quenching(Cooling), \*Phase diagrams, \*Solidification, \*Aluminum alloys, \*Manganese alloys, Microstruction, Nucleation, Crystallization, Rates(Per time), Binary alloys, Reprints, \*Rapid solidification

When an alloy is solidified rapidly, it is often thermodynamically possible for several different phases to form. Which of the phases dominates the final microstructure depends on the nucleation and growth kinetics of the several possible phases and also on the detailed thermal conditions of the specific solidification process. The effects are discussed with reference to the aluminum-manganese system, where the results of several types of experiments can be understood in terms of the strikingly different nucleation and growth behavior of several stable and metastable phases.

101.237 PB91-202945 Not available NTIS National Inst. of Standards and Technology, Gaithers-

burg, MD.
Ultrasonic Texture and Stress Measurements in Anisotropic Polycrystalline Aggregates.

Final rept. P. P. Delsanto, R. B. Mignogna, and A. V. Clark. 1990, 10p

Sponsored by Office of Naval Research, Arlington, VA. Pub. in Jnl. of the Acoustical Society of America 87, n1 p215-224 Jan 90.

Keywords: \*Acoustics, \*Ultrasonic tests, \*Metal plates, \*Anisotropy, Residual stress, Texture, Reliabiltity, Comparative evaluation, Methodology, Neutron diffraction, Strain gages, Polycrystals, Aggregates, Rayleigh waves, Time-of-flight method, Deformation, Homogeneity, Reprints.

A perturbative treatment of ultrasonic Rayleigh wave propagation is applied to investigate the case of an initally deformed metal plate, assumed to be homogeneous and to consist of an orthotropic distribution of cubic crystallites. Time-of-flight measurement tech-niques are proposed for the determination of both stress and texture. An analysis of these experimental results and a comparison with results of both ultrason-ic bulk waves and neutron diffraction techniques con-firm the reliability of this method. The special case of residual stresses is discussed in detail. Measurements of residual stresses with this technique agree with the results of strain gage measurements.

PB91-204156 Not available NTIS National Inst. of Standards and Technology (IMSE), Gaithersburg, MD. Metallurgy Div. Crystalline and Glassy Phases of Transition-Metal

Métalloid Systems. Final rept.

R. E. Watson, and L. H. Bennett. 1991, 11p Sponsored by Department of Energy, Washington, DC. Pub. in Physical Review B 43, n14 p11 642-11 652, 15

Keywords: \*Metallic glasses, \*Nickel alloys, \*Iron alloys, \*Metalloid, \*Polymorphism, Phosphorus additions, Boron additions, Silicon additions, Carbon additions, Nitrogen additions, Crystal structure, Reprints.

Glasses formed in the Ni-P and Fe-B systems are known to be polymorphic. The crystalline phases in

these systems display markedly different metalloid environments and a one-to-one relationship can be made vironments and a one-to-one relationship can be made between those environments and the glassy phases for Ni-P. It is the purpose of the present paper to explore the prospects for polymorphism in other transition-metal-rich metalloid glassy systems in which the metalloids are P, Si, B, C, and N. The known crystal structures of the phosphides, silicides, carbides, nitrides, and borides have been inspected using radical vorces (Migray Cost), cell construct to deduce me Voronoi (Wigner-Seitz) -cell constructs to deduce metalloid-site nearest-neighbor arrangements. The occurence of differences, such as those obtained in Ni-P and Fe-B, is taken as indicative of possible polymorphism in the glasses. A list of such glasses has been constructed. It is seen that polymorphism is most likely to occur in the phosphides and silicides, and very unlikely in the nitrides.

101,239

PB91-236760 Not available NTIS Mational Bureau of Standards (IMSE), Gaithersburg, MD. Metallurgy Div.

Microstructural Control Through Diffusion-Induced Grain Boundary Migration.

Final rept.

C. A. Handwerker, and J. W. Cahn. 1988, 7p Pub. in Materials Research Society Symposium Proceedings, v106 p127-133 1988.

Keywords: \*Microstructure, \*Grain boundaries, \*Diffusion, \*Metals, \*Ceramics, Migration length, Vapor deposition, Low temperature, Silicon, Process control, Polycrystals, Compositions, Reprints.

Diffusion-induced grain boundary migration (DIGM) is a Diffusion-induced grain boundary migration (DIGM) is a common, but only recently discovered low temperature phenomenon that results in high rates of both chemical mixing (or unmixing) and grain boundary migration. DIGM is found in many situations where chemical heterogeneities lead to diffusion. For example, DIGM is observed during diffusion and compound formation in polycrystalline multilayer contact systems recolled by low temperature deposition techniques. produced by low temperature deposition techniques. The diffusional mixing along the moving grain boundary is high, localized, and results in a distinctive composition profile behind the moving interface. Theory has indicated, and experiments have confirmed, which conditions lead to DIGM and which conditions suppress it. The microstructural changes can result in either a grain refinement as seen in many metallic sys-tems or in enhanced grain growth as seen in polysili-con. In either case these microstructural and composi-tional changes are controllable in a way that may allow fabrication of unique devices.

101,240

PC A04/MF A01 National Inst. of Standards and Technology (CAML), Gaithersburg, MD.

Phase-Field Phase-Field Model for Isothermal Phase Transi-

tions in Binary Alloys. A. A. Wheeler, W. J. Boettinger, and G. B. McFadden. Aug 91, 52p NISTIR-4662

Keywords: \*Binary alloys, \*Phase transformations, Copper nickel alloys, One-dimensional calculations, Two-dimensional calculations, Asymptotic methods, Interfaces, Separation.

The authors describe a new phase-field model, which models isothermal phase transitions between ideal binary alloy solution phases. Equations are developed for the temporal and spatial variation of the phase field, which describes the identity of the phase, and for the composition. The authors conduct an asymptotic analysis as the gradient energy coefficient of the phase field becomes small. From their analysis they show that their model recovers classical sharp inter-face models of this situation when the interfacial layers are thin, and they show how to relate the parameters appearing in the phase-field model to material and growth parameters in real systems. Further, the authors identify three stages of temporal evolution; the first corresponding to interfacial genesis which occurs very rapidly, the second to interfacial motion controlled by the local energy difference across the interface and by the local energy uniterline across the finite accale in which curvature effects are important, and corresponds to Ostwald ripening. The authors also present results of numerical calculations.

101,241

PB92-116938

Not available NTIS

# Nonferrous Metals & Alloys

National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Metallurgy Div.

Microstructural Studies of TI-Al Alloys In the Vicini-

ty of the 'Eutectoid' Reaction. Final rept.

S. A. Jones, R. D. Shull, A. J. McAlister, and M. J.

Kaufman. 1988, 6p Pub. in Scripta Metallurgica 22, n8 p1235-1240 Aug

Keywords: \*Binary alloys, \*Titanium alloys, \*Aluminum alloys, Phase transformations, Phase diagrams, Intermetallic compounds, Thermal analysis, Electron microscopy, High temperature tests, Eutectoids, Compositions, Reprints.

The Ti-Al phase diagram in the composition range between 35 and 50 atomic percent Al has been studied by means of optical and transmission electron microscopy and differential thermal analysis. The observations indicate inconsistencies with the alpha to alpha(2) + gamma eutectoid interpretation of the phase equilibria near 1100 C at 45 at. % Al and suggest the low temperature 'eutectoid-like' structure may be produced by the decomposition of the high temperature alpha phase via a cellular reaction: alpha (solid solution) to alpha + gamma.

### **Plastics**

PB91-148247 Not available NTIS National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Polymers Div.

Multistep Stress-Relaxation Behavior in Uniaxial Extension of an Ethylene-Hexene Copolymer. Final rept.

J. Zapas, and J. M. Crissman. 1990, 13p Pub. in Jnl. of Rheology 34, n1 p1-13 Jan 90.

Keywords: \*Polyethylene, \*Stress relaxation, \*Ethylene copolymers, \*Hexenes, Viscoelasticity, Performance prediction, Constitutive equations, Reprints.

For crystallizable polymers such as polyethylene it is found that the mechanical response in a stress relax-ation experiment is nonlinear, even at quite small deformations, and the behavior for some multistep stress relaxation strain histories cannot be described quantitatively by the BKZ theory. A better description of the behavior is obtained using a new constitutive equation proposed by Zapas. The predictions of both the BKZ theory and the new description are shown for a series of single and multistep stress-relaxation experiments done in uniaxial extension on an ethylene-hexene copolymer. The results of the calculations using the new description are in good agreement with experiment.

PB91-150086 Not available NTIS

National Inst. of Standards and Technology (NML), Boulder, CO. Chemical Engineering Science Div. Biodegradable Plastics: An Idea Whose Time Has Come.

J. D. Evans, and S. K. Sikdar. 1990, 5p Pub. in CHEMTECH 20, p38-42 Jan 90.

Keywords: \*Packaging materials, \*Plastics, \*Biodeterioration, \*Waste disposal, Enzymes, Photochemical reactions, Valeric acid, Polymers, Earth fills, Butyric acid, Reprints.

Because of severe environmental impacts of the use of plastics in recent times, regulatory and government authorities in many countries are beginning to outlaw certain plastic products, especially in packaging. Biodegradable plastics have emerged lately to redress the problems. In the article the progress made in this endeavor is reviewed and a few commercial successes are highlighted.

101,244 PB91-189712 PB91-189712 Not available NTIS National Bureau of Standards (IMSE), Gaithersburg, MD. Polymers Div. Effect of Crosslink Density on Physical Aging of

Epoxy Networks.
Final rept.
A. Lee, and G. B. McKenna. 1988, 6p
Pub. in Polymer 29, n10 p1812-1817 Oct 88.

Keywords: \*Networks, \*Crosslinking, \*Aging tests(Materials), \*Epoxy resins, Temperature dependence, Density(Mass/volume), Polyoxypropylene, Stress relaxation, Glass, Transition temperature, Specific heat, Calorimetry, Superposition(Mathematics), Thermodynamic equilibrium, Quenching(Cooling), Reprints, DGEBA.

Physical aging of different crosslink density polypropylene oxide/DGEBA networks were investigated using the small-strain stress relaxation technique in simple extension. The effects of crosslink density on the glass transition temperature, Tg, and the change in specific heat at Tg were measured using a scanning calorimeter in heating. Although an increase in Tg was observed as crosslink density increased, contrary to other studies of crosslinked polymers, the specific heat did not change as the crosslink density changed. Aging was studied at several values of temperature below Tg after quenching from above Tg. The stress relaxation curves at different aging times, temperatures and crosslink densities were able to superimtures and crosslink densities were able to superimposed to form a single master curve, demonstrating the applicability of a time-aging time-temperature-crosslink density superposition principle to this type of network. Under all aging conditions, the double logarithmic shift rate was found to decrease with increasing crosslink density while being independent of temperature for a given network. Furthermore, at temperatures of 10.0 and 5.0 below Tax the network classes were of 10 C and 5 C below Tg, the network glasses were aged into structural equilibrium.

101,245 PB91-189720 Not available NTIS National Inst. of Standards and Technology (IMSE), Gaithersburg, MD. Polymers Div. Viscoelastic Response of Epoxy Glasses Subjected to Different Thermal Treatments.

Final rept.

Final rept.

A. Lee, and G. B. McKenna. 1989, 4p

Pub. in Proceedings of ANTEC 89 Annual Technical
Conference of Society of Plastics Engineers (47th),
New York, NY., May 1-4, 1989, p1170-1173.

Keywords: \*Epoxy resins, \*Crosslinking, \*Networks, \*Viscoelasticity, Thermodynamic equilibrium, Heat treatment, Glass, Transition temperature, Polymers, Aging tests(Materials), Quenching(Cooling), Stress relaxation, Time dependence, Temperature dependence,

Density(Mass/volume), Deformation, Reprints Superposition(Mathematics), Deformation, Reprints.

Physical aging studies were made using model epoxy network glasses. Linear and nonlinear viscoelastic responses were measured after quenching the glass from above Tg to the temperature of interest. In the linear viscoelastic regime, the authors studied the effects of temperature and crosslink density on physical aging. The stress relaxation curves at different aging times, temperatures and crosslink densities were able to be superimposed to form a single master curve, to be superimposed to form a single master curve, demonstrating the validity of a time-aging time - temperature - crosslink density superposition principle for this type of epoxy network. Furthermore, at temperature of 10 C and 5 C below Tg, the network glasses were aged into structural equilibrium, thus obtaining t star, the time required to reach structural equilibrium. Results in the nonlinear viscoelastic regime showed that I star did not change with the applied stress; there-fore, aging is not 'erased' by large mechanical stimuli. These results support the argument that the volume recovery which occurs during aging impact the small deformation response differently than it does the large deformation response.

Not available NTIS PB91-189829 National Bureau of Standards (IMSE), Gaithersburg, MD. Polymers Div.

Physical Aging and the Viscoelastic Response of

Network Glasses.

Final rept.
G. B. McKenna, and A. Lee. 1988, 4p
Pub. in Proceedings of the International Conference
on Deformation, Yield and Fracture of Polymers (7th),
Cambridge, UK., April 11-14, 1988, p2/1-2/4.

Reyworus: 'Epoxy resins, 'Networks, 'Aging tests(Materials), Superposition(Mathematics), Deformation, Viscoelasticity, Glass, Transition temperature, Stress tests, Time dependence, Quenching(Cooling), Crosslinking, Reprints.

Physical aging studies were made using a model epoxy network. Linear and nonlinear viscoelastic responses were measured after quenching the glass from above Tg to temperatures near Tg. Results are presented which show that aging is not 'erased' by large mechanical deformations rather the time required for the glass to age into equilibrium is independent of the applied stress.

PB91-236612 Not available NTIS National Inst. of Standards and Technology (MSEL),

Gaithersburg, MD. Polymers Div.
Long Time Creep and Lifetime Behavior in Uniaxial
Extension of a Linear Low Density Polyethylene. Final rept.

J. M. Crissman. 1991, 7p Pub. in Polymer Engineering and Science 31, n8 p541-547 Apr 91.

Keywords: \*Polymers, \*Plastics, \*Polyethylene, Time dependence, \*Creep tests, Density, Predictions, Services life, Stress tests, Temperature dependence, Graphic methods, Reprints.

The paper describes uniaxial creep measurements done on a linear low density polyethylene over a wide range of temperatures and applied stresses. It is found that the creep behavior overall is quite complex and that the one quantity which can best be used to predict useful lifetime of this material is the time at which necking is observed. The time to neck data has been used to generate a composite curve which can serve as an upper bound to lifetime prediction.

# **Wood & Paper Products**

DE91007688 PC A05/MF A01 National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Center for Chemical Engineering. Advanced sensor development program for the pulp and paper Industry. Final report.
Progress rept.
J. D. Allen, S. R. Charagundla, A. Macek, H. G.

Semerjian, and J. R. Whetstone. Oct 90, 100p DOE/ CF/40748-T1

Contract Al01-85CE40748

Sponsored by Department of Energy, Washington, DC.

Keywords: Emission Spectra, Flames, \*Paper Industry, \*Sodium, Absorption, Boilers, \*Combustion Control, \*Emission Spectroscopy, Hydroxyl Radicals, Mathematical Models, Measuring Instruments, Potassium, Probes, Progress Report, Radicals, Remote Sensing, Research Programs, Spent Liquors, Temperature Measurement, Windows, EDB/320300, EDB/440500, \*Aircellution control or with the control of the control \*Air pollution control equipment.

This report describes experimental and theoretical studies toward development of a remote sensing technique for non-intrusive temperature measurement based on optical spectroscopic analysis of recovery boiler. The overall objectives were (a) construction of a fiber-optic system for measurement of spectroscopic emission intensities at several wavelengths and (b) deemission intensities at several wavelengths and (b) de-velopment of a computer program relating these inten-sities to temperatures of the emitting species. The emitting species for temperature measurements in flames can be either naturally occurring free radicals (OH, CH, C(sub 2)) or atoms which, in turn, can be either naturally occurring or seeded into flames. Sodium atoms, the obvious emitters in recovery boil-ers, are not promising as thermometric species be-cause of their high concentration. At high concentracause of their high concentration. At high concentra-tions, strong self-absorption results cause optical depths to be much smaller than the sampling depths desired for recovery boilers. An experimental program was, therefore, undertaken with the objective of identification and spectroscopic detection and measurement of other naturally occurring thermometric species. The program consisted of several laboratory studies and four field trips to different recovery boilers. 19 refs., 43 figs., 8 tabs.

### General

101,249 PB91-147546

Not available NTIS

### General

National Bureau of Standards (NML), Gaithersburg, MD. Office of Standard Reference Data.

Factual Materials Databanks - The Need for Standards.

Final rept.

H. Krockel, K. Reynard, and J. Rumble. 1987, 60p Pub. in VAMAS (Versailles Project on Advanced Materials and Standards) Report, pi-51 Jul 87.

Keywords: \*Materials, \*Data bases, \*Standards, Information systems, Data analysis, Access, Reprints, National Institute of Standards and Technology.

The VAMAS Task Group on Factual Materials Databanks has identified the areas where standards development would significantly and positively impact the building and dissemination of materials databanks. Materials databanks are becoming substantial ele-ments of the computerized flow of information on materials properties from the generation of the information to its use. Their features and operational conditions will therefore be influenced by all standards related to any phase of the information flow. Accordingly, the review includes the aspects of data generation, data anlysis, data presentation, access to data, and use of data; and the report presents sets of recom-mendations under four headings: Basic considerations for handling data; Material data generation and reporting; Materials databanks; and Access to materials

101.250

PB91-148049
Not available NTIS
National Inst. of Standards and Technology (NML),
Boulder, CO. Chemical Engineering Science Div.
Apparatus for Measurement of Coefficient of Fric-

A. J. Slifka, J. D. Siegwarth, L. L. Sparks, and D. K. Chaudhuri. 1990, 7p

Sponsored by National Aeronautics and Space Administration, Huntsville, AL. George C. Marshall Space Flight Center.

Pub. in Advances in Cryogenic Engineering (Materials) 36, p1119-1125 1990.

Keywords: \*Coefficient of friction, \*Friction measurement, Controlled atmospheres, Cryogenics, Steels,

An apparatus has been built at the National Institute of Standards and Technology in Boulder, Colorado to measure the coefficient of friction in certain controlled atmospheres. The machine uses either of two configurations of specimens. A cone-on-cone configuration can be loaded to produce a contact stress of 137 MPa (20 ksi) and surface velocities from 0.03 m/s to 1.2 m/s. A ball-on-flat configuration can be loaded to produce a Hertzian contact stress in excess of 1830 MPa (267 ksi) and surface velocities from 0.06 m/s to 2.0 m/s. The designed temperature-range of operation is 80 to 1030 K. The machine is described and some test results are presented.

101,251 PB91-204040 Not available NTIS National Inst. of Standards and Technology (IMSE), Gaithersburg, MD.

International Collaboration in Prestandards Research on Advanced Materials within the Context of VAMAS.

Final rept.

L. H. Schwartz, and B. W. Steiner. 1989, 6p Pub. in ASTM (American Society for Testing and Materials) Standardization News 17, n2 p28-33 Feb 89.

Keywords: \*Materials tests, \*Data bases, \*Standards, \*Research projects, \*International cooperation, Surface chemistry, Chemical analysis, Characterization, Ceramics, Polymer matrix composites, Methodology, Cryogenics, Superconductors, Wear, Corrosion, Weldments, Creep tests, Fracture mechanics, Fatigue, Reprints, \*Vamas(Versailles Project on Advanced Materials and Standards).

VAMAS, the Versailles Project on Advanced Materials and Standards, now encompasses international collaboration in thirteen areas of prestandards research on advanced materials. One of the most successful projects has stimulated the development of a consensus on high priority action essential for the development of compatible computerized materials data-banks. Another has established a framework for a coherent international research effort laying the foundation for standards in surface chemical analysis. Six projects address critical problem areas in the characterization of particular classes of advanced materials:

ceramics, polymer blends, polymer composites, efficient test procedures for polymer properties, super-conducting and cryogenic structural materials, and bioengineering materials. The other five projects deal with characterization of the response of advanced materials to particularly challenging performance situations: wear, hot salt corrosion resistance, weld characteristics, creep crack growth, and low cycle fatigue. Recent results of VAMAS activity in these various areas are surveyed and directions for the future are

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PC A05/MF A01 PB92-126424 National Inst. of Standards and Technology (MSEL), Gaithersburg, MD.

Materials Reliability. Technical Activities, 1991. (NAS-NRC Assessment Panel, February 13-14, 1992).

H. I. McHenry. 1992, 95p NISTIR-4695 See also PB91-143339.

Keywords: \*Materials, \*Research projects, Quality, Reliability, Safety, Process control, Nondestructive tests, Standards, Cryogenics, Automation, Fracture mechanics, Metals, Microstructure, Physical properties, Ceramics, Superconductors, Advanced materials, Intelligent welding, Acoustic microscopy.

The report describes the 1991 fiscal-year programs of the Materials Reliability Division of the Materials Science and Engineering Laboratory. It summarizes the principal accomplishments in three general research areas: materials performance, properties, and processing. The Fracture Mechanics, Fracture Physics, Nondestructive Evaluation, and Composite Materials Groups work together to detect damage in metals and composite materials and to assess the significance of the damage with respect to service performance. The Cryogenic Materials and Physical Properties Groupsinvestigate the behavior of materials at low temperature and measure and model the physical properties of advanced materials, including composites, ceramics, and the new high-critical-temperature superconductors. The Welding and Thermomechanical Processing Groups investigate the nonequilibrium metallurgical changes that occur during processing and affect the quality, microstructure, properties, and performance of

101,253

PC A15/MF A03 PB92-126606 National Inst. of Standards and Technology (MSEL), Gaithersburg, MD.

National Educators Workshop: Update '90. Standard Experiments in Engineering Materials Science and Technology.

Final rept.

J. S. Harris, and J. A. Jacobs. Nov 91, 341p NIST/ SP-822

Also available from Supt. of Docs as SN003-003-03124-1. See also N90-24350 and N91-20207. Proceedings of a Workshop held in Gaithersburg, MD., November 13-15, 1990. Prepared in cooperation with Norfolk State Univ., VA., and National Aeronautics and Space Administration, Washington, DC. Sponsored by ASM International, Detroit, MI., and Battelle Pacific Northwest Labs., Richland, WA.

Keywords: \*Education, \*Materials tests, \*Fracture(Mechanics), \*Structural properties, Standards, Microstructure, Steels, Metals, Strain rate, Fiber reinforced composites, Ceramics, Tensile properties, Metals, et al., \*Link Properties, Tensile pro Metal working, Thermoplastics, Biodegradation, Universities, Experimentation.

The report includes proceedings of a workshop sponsored jointly by NIST and the Schools of Technology and Science, Norfolk State University, Norfolk, Virginia, and held in Gaithersburg, Maryland, November 13-15, 1990. The workshop theme was strengthening materials education. Material in the publication can serve as a valuable guide to faculty who are interested in useful experiments for their students. There was a blend of experiments on new materials and traditional materials. Uses of computers in MS&E, experuimental design and an approach to systematic materials are among the topics presented.

# **MATHEMATICAL SCIENCES**

### Algebra, Analysis, Geometry, & Mathematical Logic

101,254 PB91-147850 Not available NTIS
National Inst. of Standards and Technology (NEL),
Gaithersburg, MD. Scientific Computing Div.
Computing the Eigenvalues and Eigenvectors of Symmetric Arrowhead Matrices.

Final rept. D. P. O'Leary, and G. W. Stewart. 1990, 9p Pub. in Jnl. of Computational Physics 90, n2 p497-505 Oct 90.

Keywords: \*Sparse matrix, \*Matrices, Fermi liauids, Eigenvectors, Eigenvalues, Radiationless decay, Computation, Algorithms, Reprints.

The paper treats the eigenvalue problem for a symmetric matrix which is zero except for its main diagonal and one row and column. Such problems arise in the description of radiationless transitions in isolated molecules and of oscillators vibrationally coupled with a Fermi liquid. In these applications, the order of the matrix A can be in the thousands. The purpose of the paper is to present formulas and efficient algorithms for computing eigenvalues and eigenvectors of such matrices.

101.255

Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Quantum Physics Div.

Asymptotic Shooting Method for the Solution of Differential Equations.

Final rept.

A. Holubec, A. D. Stauffer, P. Acacia, and J. A. Stauffer. 1990, 15p
Pub. in Jnl. of Physics A: Mathematical and General 23, p4081-4095 1990.

Keywords: \*Differential equations, Numerical integration, Analytic continuation, Asymptotic methods, Series(Mathematics), Polynomials, Eigenvalues, Re-

The authors present a method for the solution of ordinary differential equations over a semi-infinite interval, including the determination of eigenvalues, which is in principle capable of arbitrary accuracy. The solution is expressed in terms of finite polynomials, rendering the integration or determination of zeros of such solutions a straightforward matter. The authors have applied the method to a number of examples including the determination of the eigenvalues of the screened Coulomb potential and the three-dimensional quartic oscillator.

Not available NTIS PB91-148759

Not available NTIS
National Inst. of Standards and Technology (NML),
Gaithersburg, MD. Ionizing Radiation Div.
Certain Theorems on Bilateral Generating Functions Involving Hermite, Laguerre, and Gegenbauer Polynomials. Final rept.

7. H. Hubbell, and H. M. Srivastava. 1990, 11p Pub. in Jnl. of Mathematical Analysis and Applications 152, p343-353 1990.

Keywords: \*Generating functions, Hermite polynomials, Laguerre polynomials, Bessel functions, Gamma transport theory, Theorems, Reprints, Gegenbauer polynomials, Konhauser polynomials.

The object of the paper is to present simpler proofs of the various generalizations of some interesting results on bilateral generating functions which were derived recently by group-theoretic methods. It is also shown how one of our main theorems on generating functions would apply not only to the Bessel function but indeed also to the Konhauser biorthogonal polynomials whose special case when s=2 was encountered in

# Algebra, Analysis, Geometry, & Mathematical Logic

certain analytical calculations involving the penetration of gamma rays through matter.

101,257 PB91-159046 Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Mathematical Analysis Div. Simplified Error Bounds for Newton's Rule.

Final rept. F. W. J. Olver. 1986, 7p

Pub. in IMA Jnl. of Numerical Analysis 6, n3 p373-379

Keywords: \*Iterative methods, \*Newton method, Roots of equations, Error analysis, Analytic functions, Approximation, Precision, Reprints, Interval analysis.

A posteriori error bounds are given for approximations to zeros of a function f obtained by Newton's rule. Here f is a differentiable function of a real variable, or an analytic function of a complex variable. The bounds are somewhat simpler and sharper than existing results. Numerical examples are included.

101,258 PB91-175281 Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Mathematical Analysis Div. Some Algorithms for Approximating Convolutions.

Final rept.
D. P. O'Leary. 1988, 13p
Pub. in Computer Vision, Graphics, and Image Processing 41, n3 p333-345 Mar 88.

Keywords: \*Image processing, \*Convolution, Parallel processing, Factorization, Polynomials, Algorithms, Reprints, Singular value decomposition.

The paper presents some algorithms for approximating two-dimensional convolution operators of size n x n, n odd, by a product, or sum of products, of 3 x 3 convolutions. Inaccuracies resulting from the approximation as well as from fixed point computation are discussed, and examples are given.

101,259 PB91-187245 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Applied and Computational Mathematics Div.

Algorithms for Special Tridiagonal Systems.

Final rept. R. F. Boisvert. 1991, 20p Pub. in SIAM (Society for Industrial and Applied Mathematics) Jnl. on Scientific and Statistical Computing 12, n2 p423-442 Mar 91.

Keywords: \*Matrices, Elliptic differential equations, Poisson equation, Fourier analysis, Factorization, Algorithms, Reprints, \*Tridiagonal matrices.

Algorithms for the solution of symmetric diagonally dominant tridiagonal systems of linear equations with constant diagonals are considered. Such systems occur, for example, when solving certain constant-coefficient elliptic partial differential equations by the Fourier method. In particular, the specialized LU factorization method of Malcolm and Palmer (SpLU), the special conduction method of Malcolm and Palmer (SpLU), the special conduction method of Malcolm and Palmer (SpLU), the cyclic reduction method of Hockney (CR), and the reversed triangular factorization method of Evans (RTF) are considered. An interesting property of the first two algorithms is that they may be terminated early for highly diagonally dominant systems. A new implementation of RTF that also has the property is presented, significantly reducing its operation count in many cases. The slightly perturbed systems that arise from problems with Neumann or periodic boundary conditions are also considered, with extensions given for SpLU to the periodic case and RTF to the Neumann case. Floating-point operation counts are given for each method, and the results of experiments on a single scalar processor are reported.

101,260 PB91-187799 PB91-187799 PC A03/MF A01 National Inst. of Standards and Technology (NEL), Gaither Burg, MD. Applied and Computational Mathe-

Convergence Properties of a Class of Rank-Two

Updates. P. T. Boggs, and J. W. Tolle. Apr 91, 49p NISTIR-4554

Contracts AFOSR-ISSA-90-0004, AFOSR-88-0267 Prepared in cooperation with North Carolina Univ. at Chapel Hill. Sponsored by Air Force Office of Scientific Research, Bolling AFB, DC.

Keywords: \*Numerical analysis, Mathematical programming, Sequences(Mathematics), Newton method, Approximation, Iteration, Convergence, Matrices, Theorems, \*Foreign technology, Unconstrained optimization, Constrained optimization.

Many optimization algorithms generate, at each iteration, a pair x sub k, H sub k consisting of an approximation to the solution, x sub k, and a Hessian matrix approximation, H sub k, which contains local secondorder information about the problem. Much is known about the convergence of the x sub k to the solution of the problem but relatively little about the behavior of the problem but relatively little about the behavior of the sequence of matrix approximations. The authors analyze the sequence H sub k generated by the extended Broyden class of updating schemes independ-ently of the optimization setting in which they are used, deriving various conditions under which convergence is assured and delineating the structure of the limits. Rates of convergence are also obtained. The results extend and clarify those already in the literature.

101,261
PB91-203497
Not available NTIS
National Inst. of Standards and Technology (NML),
Gaithersburg, MD.
Nature of Collinearity.

Final rept.

J. Mandel. 1989, 9p Pub. in Jnl. of Quality Technology 21, n4 p268-276 1989

Keywords: \*Collinearity, Regression analysis, Quality control, Reprints, Multiple linear regression, Effective prediction domain, Singular value decomposition.

Collinearity is treated as an indication that use of the regression equation for prediction is limited to a specific portion of the sample space regressors. A method is presented for determination of this portion, called the Effective Prediction Domain (EPD). The same basic technique is also used for the detection of collinearity. Numerical examples are discussed in detail.

101,262 PB91-216754

(Order as PB91-216705, PC A07/MF A01) National Inst. of Standards and Technology, Gaithers-

burg, MD.
Root Projection of One-Sided Time Series.

J. A. Simmons. 1991, 11p Included in Jnl. of Research of the National Institute of Standards and Technology, v96 n3 p333-343 May/Jun

Keywords: \*Time series analysis, \*Signal processing, Least squares method, Laplace transformation, Complex variables, Prony method, Gram-Schmidt algorithm, Root projection, Deconvolution.

Until recently it has been impossible to accurately determine the roots of polynomials of high degree, even for polynomials derived from the Z transform of time series where the dynamic range of the coefficients is generally less than 100 dB. In a companion paper, two new programs for solving such polynomials were dis-cussed and applied to signature analysis of one-sided time series. The author presents here another technique, that of root projection (RP), together with a Gram-Schmidt method for implementing it on vectors of large dimension. This technique uses the roots of the Z transform of a one-sided time series to construct a weighted least squares modification of the time series whose Z transform has an appropriately modifed root distribution. Such a modification can be employed in a manner which is very useful for filtering and deconvolution applications. Examples given here include the use of boundary root projection for front end noise reduction, and a generalization of Prony's method.

101,263 PB91-216762

(Order as PB91-216705, PC A07/MF A01) National Inst. of Standards and Technology, Gaithers-

Deconvolution of Acoustic Emission and Other Causal Time Series.

J. A. Simmons. 1991, 25p
Included in Jnl. of Research of the National Institute of Standards and Technology, v96 n3 p345-369 May/Jun

Keywords: \*Time series analysis, \*Signal processing, \*Acoustic emissions, Fast Fourier transforms, One dimensional, Transducers, Calibration, Comparison, Algorithms, Graphs(Charts).

A new technique, root projection (RP), is given for quantitative deconvolution of causal time series in the presence of moderate amounts of noise. Deconvolution is treated as a well-conditioned but underdetermined problem and a priori information is employed to obtain comparable noise reduction to that achieved by singular value decomposition (SVD) techniques while providing more accurate frequency information about the inverse. Two detailed examples are given. The first gives noise analysis for alternate methods for deconvolution with a Gaussian kernel. The second example presents a model acoustic emission transducer calibration problem with typical noisy and incomplete output data. This example is treated by the use of a robust cross-cutting algorithm combining both the RP and SVD methods.

101,264

PB92-112408 PC A09/MF A02 National Inst. of Standards and Technology (CAML), Gaithersburg, MD.

NBS-INA. The Institute for Numerical Analysis. UCLA 1947-1954.

Special pub. (Final).

M. R. Hestenes, and J. Todd. Aug 91, 185p NIST/ SP-730

Also available from Supt. of Docs. as SN003-003-03094-5. Prepared in cooperation with California Univ., Los Angeles. Dept. of Mathematics, and California Inst. of Tech., Pasadena. Dept. of Mathematics. Sponsored by Mathematical Association of America, Washinaton, DC.

Keywords: Differential equations, Numerical integration, Numerical analysis, Digital computers, Computer applications, Linear programming, Historical aspects, Matrices, US NBS, \*Institute for Numerical Analysis,

The report is a history of the Institute for Numerical Analysis (INA) with special emphasis on its research program during the period 1947 to 1956. The Institute for Numerical Analysis was located on the campus of the University of California, Los Angeles. It was a section of the National Applied Mathematics Laboratories. which formed the Applied Mathematics Division of the National Bureau of Standards (now the National Institute of Standards and Technology), under the U.S. Department of Commerce. The history of the program at INA is concerned primarily with the development of mathematics pertinent to solving numerical computations. The development could happen only if some mathematicians were proficient in handling the electronic digital computers. To insure that there would be some, INA was constituted. It was well funded, and could attract first class mathematicians to take a year off for research at INA. They were in the midst of people solving problems of considerable difficulty using digital computers. They were thus enticed into using them. When this happened, many important developments emerged. The history is centered around these people and discusses who they were, what their interests were, and what they did.

101,265

PB92-123108 PC A03/MF A01 National Inst. of Standards and Technology (CAML), Gaithersburg, MD. Applied and Computational Mathematics Div.

Computing Delaunay Triangulations for Comet-Shaped Polygons. J. Bernal. Nov 91, 19p NISTIR-4716

See also PB89-129480.

Keywords: \*Computational geometry, Computation, Polygons, Algorithms, \*Delauney triangulations, Computational complexity, Voronoi diagrams.

The author presents two triangulation algorithms which combined produce an algorithm for computing Delaunay triangulations for comet-shaped polygons. The first algorithm constructs in linear time a triangulation for a comet-shaped polygon. The second algo-rithm constructs a Delaunay triangulation for a polygon from any triangulation for the polygon. The algorithms can be used for deleting vertices in a Delaunay triangulation and for computing constrained Delaunay triangulations.

### MATHEMATICAL SCIENCES

### Operations Research

### **Operations Research**

101,266 PB91-148775

Not available NTIS National Bureau of Standards (NEL), Gaithersburg,

MD. Center for Applied Mathematics.
Second Order Sensitivity Analysis in Factorable Programming: Theory and Applications.

Final rept.

R. H. F. Jackson, and G. P. McCormick. 1988, 273p Pub. in Mathematical Programming 41, n1 p1-273 May

Keywords: \*Mathematical programming, \*Optimization, Nonlinear programming, Tensors, Reprints, Second-order sensitivity analysis.

Second-order sensitivity analysis methods are developed for analyzing the behavior of a local solution to a constrained nonlinear optimization problem when the problem functions are perturbed slightly. Specifically, formulas involving third-order tensors are given to compute second derivatives of components of the local solution with respect to the problem parameters. When in addition, the problem functions are factorable, it is shown that the resulting tensors are polyadic in nature.

101.267

Not available NTIS PB91-174540 National Bureau of Standards (NEL), Gaithersburg, MD. Mathematical Analysis Div.

Applications of Operations Research Techniques to System Design and Evaluation.

Final rept. R. E. Chapman. 1986, 2p

Pub. in Proceedings of Symposium on ASME (American Society of Mechanical Engineers) Codes and Recent Advances in PVP and Valve Technology, Chicago, IL., July 20-24, 1986, p139-140.

Keywords: \*Systems design, \*Systems analysis, \*Operations research, Systems engineering, Economic analysis, Mathematical programming, Monte Carlo methods, Simulation, Mathematical models, Reprints.

The paper illustrates how several operations research the paper litustrates now several operations research techniques can be used to facilitate the system design/evaluation process. Two classes of techniques, mathematical programming and Monte Carlo simulation, are used to demonstrate how cooperative efforts between engineering professionals and operations research analysts can promote more informed decision making. The paper concludes with a discussion of the role of standardized practices for performing economic evaluations of competing system designs.

101.268

PB91-174896 Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Operations Research Div.
State-of-the-Art of Computational Testing of Math-

ematical Programming Algorithms.

Final rept.
R. H. F. Jackson. 1985, 6p
Pub. in Mathematical Programming Society Committee on Algorithms Newsletter, n12 p8-13 May 85.

Keywords: \*Mathematical programming, Algorithms, Tests, Computer program verification, Reprints, \*Computational testing.

The article summarizes some of the philosophical aspects on computational testing, including some historical background.

PC A03/MF A01 PB91-187815 National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Applied and Computational Mathematics Div.

Interior-Point Method for Linear and Quadratic

Programming Problems.
P. T. Boggs, P. D. Domich, J. E. Rogers, and C. Witzgall. Apr 91, 13p NISTIR-4556

Keywords: \*Linear programming, \*Ouadratic programming, Mathematical programming, Algorithms, Interior point methods.

The authors have been working on a particular class of interior point methods for solving linear programming problems for several years. The methods combine several search directions that are readily computed at each iteration. The final step is then calculated by computing the step that solves the original problem restricted to the subspace spanned by these several di-rections. In the paper, they propose an extension of these ideas to the case of convex quadratic program-

101 270

PB91-204198 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Applied and Computational Mathematics Div.

Convergence Behavior of Trajectories for Linear Programming.

Final rept.

C. Witzgall, P. T. Boggs, and P. D. Domich. 1990,

Contract ONR-N-0014-87-F0053
Sponsored by Office of Naval Research, Arlington, VA Pub. in Contemporary Mathematics 114, p161-187 1990.

Keywords: \*Linear programming, \*Trajectories, \*Convergence, Linear inequalities, Logarithm functions, Constraints, Reprints, Analytic centers, Center mani-

The convergence behavior of center trajectories arising from the use of the logarithmic barrier function in linear programming is examined based on the concept of analytic center of a system of linear constraints. Main results are the convergence of A-trajectories to g-centers of the optimal face and the convergence of their tangential directions. Both results hold in the presence of primal and dual degeneracies. g-center varieties are introduced extending the concept of analytic g-centers.

101.271

PB92-116318 PC A03/MF A01 National Inst. of Standards and Technology (CAML), Gaithersburg, MD.

Merit Function for Inequality Constrained Nonlinear Programming Problems. P. T. Boggs, J. W. Tolle, and A. J. Kearsley. Oct 91, 34p NISTIR-4702

See also PB90-123944 and PB86-105830. Prepared in cooperation with North Carolina Univ. at Chapel Hill. Dept. of Mathematics, and Rice Univ., Houston, TX. Dept. of Mathematical Sciences.

Keywords: \*Nonlinear programming, Optimization, Ouadratic programming, Constraints, Convergence, Algorithms, Tables(Data), \*Merit functions.

The authors consider the use of the sequential quad-The authors consider the use of the sequential quadratic programming (SOP) technique for solving the inequality constrained minimization problem min sub x f(x) subject to:  $g(sub\ i)(x) < or = 0$ , i = 1,..., m. SOP methods require the use of an auxiliary function, called a merit function or line-search function, for assessing the steps that are generated. The authors derive a merit function by adding slack variables to create an equality constrained problem and then using the merit function developed earlier by the authors for the equality constrained case. They stress that they do not solve the slack variable problem, but only use it to construct the merit function. The resulting function is simplified in a certain way that leads to an effective procedure for updating the squares of the slack variables. The final form of the merit function has many desirable properties, and is demonstrated to be effective in prac-

### Statistical Analysis

101,272 PB91-147017 PB91-147017 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Applied and Computational Mathe-matics Div. matics Div.

Orthogonal Distance Regression. Final rept.

P. T. Boggs, and J. R. Donaldson. 1989, 12p See also PB90-151747.

Pub. in Proceedings of Summer Research Conference on Contemporary Mathematics, Arcata, CA., June 10-16, 1989, v112 p183-194 1990.

Keywords: \*Error analysis, Maximum likelihood estimation, Confidence limits, Computation, Computer ap-

plications, Reprints, \*Orthogonal distance regression, Parameter estimation, Covariance matrices.

Orthogonal distance regression (ODR) is the name given to the computational problem associated with finding the maximum likelihood estimators of parameters in measurement error models in the case of nor-mally distributed errors. The authors examine the stable and efficient algorithm of Boggs, Byrd, and Schnabel (1987) for finding the solution to the problem when the underlying model is assumed to be nonlinear in both the independent variable and the parameters. The authors also describe the associated public-domain software package, ODRPACK. The authors then review the results of a simulation study that compares ODR with ordinary least squares (OLS). The authors thors also present the new results of an extension to the study. Finally the authors discuss the use of the asymptotic covariance matrix for computing confidence regions and intervals for the estimated parameters. Their conclusions are that ODR is better than OLS for the criteria considered, and that ODRPACK can provide effective solutions and useful statistical information for nonlinear ODR problems.

PB91-149443 Not available NTIS National Bureau of Standards (NEL), Boulder, CO. Sta-Not available NTIS tistical Engineering Div.

Linear Calibration When the Coefficient of Variation Is Constant.

Final rept.

Y. C. Yao, and D. F. Vecchia. 1988, 13p Pub. in Probability and Statistics, p297-309 1988.

Keywords: \*Calibrating, \*Coefficient of variation, Parameter identification, Maximum likelihood estimates, Reprints, Pitman closeness.

The report considers point estimation of the unknowns in the calibration problem when the calibration curve is a straight line through the origin and the responses are normal with variances proportional to the square of their mean. It presents four different estimators and compares their performances using the criterion of Pitman closeness. For all the practical ranges of parameter values, one of these estimators is found to dominate the others under the normality assumption. Non-normal cases are not considered.

101.274

PB91-158824 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Statistical Engineering Div. Design and Analysis of Experiments. Final rept.

J. S. Hunter, M. G. Natrella, E. H. Barnett, W. G. Hunter, and T. L. Koehler. 1988, 81p Pub. in Juran's Quality Control Handbook, Section 26, p26.1-26.81 1988.

Keywords: \*Experimental design, Factorial design, Block design, Laboratory tests, Mixtures, Statistics, Reprints.

The chapter outlines some general considerations in planning experiments and some tools for sound experimentation. Various statistical experiment designer classified according to their structure, their purpose, and the kind of information obtained. Detailed explanations of the design structure and analysis are explanations of the design structure and analysis are given for completely randomized designs, various kinds of block designs, factorial and fractional fractorial designs, and mixture designs. Some methods for planning the size of the experiment, and for planning interlaboratory tests are also given.

101,275 PB91-158907 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Statistical Engineering Div. New Yorker in Japan.

Final rept. W. Liggett. 1990, 2p Pub. in Industrial Science and Technology 31, p46-47 1990

Keywords: Culture(Social sciences), United States, Japan, Travel, Statistics, Reprints, \*National Research Laboratory of Metrology, US NIST.

A personal note is provided on experiences at NRLM (National Research Laboratory of Metrology) in Japan, which relate NIST to NRLM, and U.S. culture to that of Japan.

# Statistical Analysis

101.276

PB91-158931 Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Statistical Engineering Div.
Calibration with Working Standards.

Final rept.

T. Lwin, and C. H. Spiegelman. 1986, 6p Contract ONR-00014-83-005 Sponsored by Office of Naval Research, Arlington, VA. Pub. in Applied Statistics 35, n3 p256-261 1986.

Keywords: \*Calibration, Error analysis, Regression analysis, Nonparametric statistics, Reprints, Working standards

Certified values of working standards used for calibra-tions are rarely exact, and calibration curve procedures should take into account all sources of error, including errors in the working standards. When the errors in working standards have a known finite bound, the authors give an easily implementable accurate calibration curve procedure. It produces conservative confidence intervals based on an expansion.

101,277 PB91-203414 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Statistical Engineering Div. Estimators for Censored (Log)Normal Samples. Final rept.

J. A. Lechner. 1989, 7p

Pub. in Proceedings of Annual Reliability and Maintain-ability Symposium, Atlanta, GA., January 24-26, 1989, p262-268.

Keywords: Life tests, Reliability, Reprints, \*Lognormal distribution, Parameter estimation.

The paper presents an evaluation of the properties of several estimators of the parameters of the (two-parameter) logNormal distribution, for sample sizes from 10 to 60 and for right-censoring of 0 to 80% of the sample. Correction factors to reduce bias and recom-mendations are included. The estimators are also applicable to right-censored Normal samples.

101,278

PB91-507954 National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Statistical Engineering Div. OMNITAB 80 (ASCII): An Interactive System for Statistical and Numerical Data Analysis (Version

7.0).

Software.

Software.

Mar 91, mag tape NIST/SW/MT-91/011

System: SUN/UNIX; VMS V4.7 operating system. Language: TAR UNIX command FO. Other formats available as PB91-507962 (UNIX).

Available in 9-track, ASCII character set, 1600 or 6250 bpi. For 6250 bpi, the price is T06. Documentation included; may be ordered separately as PB87-172235.

Keywords: \*Software, \*Statistical analysis, \*Numerical analysis, \*Data analysis, Computer calculations, Computation, Tabulation processes, Integrated systems, Interactive systems, Batch processing, Regression analysis, Correlation, Magnetic tapes.

OMNITAB 80 is a high-level integrated general purpose programming language and statistical software computing system. The system enables the user to use a digital computer to perform statistical and numerical data analysis without having any prior knowledge of computers or programming language. It permits one to perform arithmetic, complex arithmetic, trigonometric calculations as well as data manipulation, special function calculations, statistical analysis, and matrix and array operations. The system responds to simple instructions to obtain accurate results since to simple instructions to obtain accurate results since reliable, varied, and sophisticated algorithms for data analysis and manipulation are referenced. It may be used either interactively or in batch mode. Some of the major statistical capabilities are regression, correlation analysis and oneway/twoway analysis. OMNITAB 80 has been installed nationally and internationally. The source language of the system is in FORTRAN for implementation on the VAX computer. Input/output is done in ASCII format. A load and run module is also included as well as a module of test problems.

PB91-507962 **CP T06** National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Statistical Engineering Div. OMNITAB 80 (UNIX): An Interactive System for Statistical and Numerical Data Analysis. Version 7.0.

Software.

May 91, mag tape NIST/SW/MT-91/012 System: SUN/UNIX; VMS V4.7 operating system. Language: TAR UNIX command FO. Other formats avail-

able as PB91-507954 (ASCII).

Available in 9-track, ASCII character set, 1600 or 6250 bpi. For 6250 bpi, the price is T06. Documentation included; may be ordered separately as PB87-172235.

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OMNITAB 80 is a high-level integrated general purpose programming language and statistical software computing system. The system enables the user to use a digital computer to perform statistical and numerical data analysis without having any prior knowledge of computers or programming language. It permits one to perform arithmetic, complex arithmetic, trigonometric calculations as well as data manipula-tion, special function calculations, statistical analysis, and matrix and array operations. The system responds to simple instructions to obtain accurate results since reliable, varied, and sophisticated algorithms for data analysis and manipulation are referenced. It may be analysis and manipulation are referenced. It may be used either interactively or in batch mode. Some of the major statistical capabilities are regression, correlation analysis and oneway/twoway analysis. OMNITAB 80 has been installed nationally and internationally. The source language of the system is in FORTRAN for implementation on the VAX computer. Input/output is done in UNIX format. A load and run module is also included as well as a module of test problems.

101,280 PB92-126671

(Order as PB92-126614, PC A06/MF A02) National Inst. of Standards and Technology, Gaithersburg, MD.

Taguchi's Orthogonal Arrays Are Classical Designs of Experiments.
R. N. Kacker, E. S. Lagergren, and J. J. Filliben.

1991, 15p

Included in Jnl. of Research of the National Institute of Standards and Technology, v96 n5 p577-591 Sep/Oct

Keywords: \*Experimental design, Factorial design, Matrices, \*Orthogonal arrays, Taguchi arrays.

Taguchi's catalog of orthogonal arrays is based on the mathematical theory of factorial designs and difference sets developed by R. C. Bose and his associates. These arrays evolved as extensions of factorial designs and latin squares. The paper (1) describes the structure and constructions of Taguchi's orthogonal arrays, (2) illustrates their fractional factorial nature, and (3) points out that Taguchi's catalog can be expanded to include orthogonal arrays developed since 1960.

101,281 PB92-126705

(Order as PB92-126614, PC A06/MF A02) Birsa Agricultural Univ., Ranchi (India). Dept. of Statis-

tics.
List of New Group Divisible Designs.

K. Sinha. 1991, 3p Included in Jnl. of Research of the National Institute of Standards and Technology, v96 n5 p613-615 Sep/Oct

Keywords: \*Experimental design, \*Block design, Tables(Data).

Group divisible designs are the most important class of partially balanced incomplete block (PBIB) designs. A list of new group divisible designs with r, k e or < 10 is provided.

### General

101,282 PB91-132175 PC A03/MF A01 National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Applied and Computational Mathematics Div.

Guide to Available Mathematical Software Problem

Classification System.
R. F. Boisvert, S. E. Howe, and D. K. Kahaner. Nov 90, 33p NISTIR-4475 See also PB90-216508.

Keywords: \*Applications of mathematics, \*Classifications, Subject indexing, Cataloging, Mathematical models, \*Computer software, Computer calculations.

A vast collection of reusable mathematical and statistical software is now available for use by scientists and engineers in their modeling efforts. This software represents a significant source of mathematical expertise, created and maintained at considerable expense. Unfortunately, the collection is so heterogeneous that it is a tedious and error-prone task simply to determine what software is available to solve a given problem. In mathematical problem-solving environments of the future such questions will be fielded by expert software advisory systems. One way for such systems to systematically associate available software with the prob-lems they solve is to use a problem classification system. The paper describes a detailed tree-structured problem-oriented classification system appropriate for such use.

# MEDICINE & BIOLOGY

# **Biochemistry**

101.283 PB91-134544 Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Chemical Engineering Science Div. Chitin-Chitosan Membranes: Separations of Amino Acids and Polypeptides.

Final rept.

D. Steward. 1990, 16p

Pub. in Annals of the New York Academy of Sciences 589, p229-244, 20 May 90.

Keywords: \*Adsorption, \*Amino acids, \*Peptides, \*Chitins, \*Membranes, Measurement, Yeasts, Alcohol oxidoreductases, Dehydrogenase, Mixtures, Permeability, Molecular weight, Diffusion theory, Crosslinking, Aldehydes, Gels, Reprints, \*Separation processes, Chitosan, Glutaraldehyde.

The permeation of several amino acids and yeast alcohol dehydrogenase (YADH) has been measured for membranes made from poly(N-acetyl-D-glucosamine)/poly(D-glucosamine)(chitin/chitosan) membranes. Sorption data for a number of amino acids has also been measured and indicates that those with polar aromatic residues are preferentially sorbed. Preferential sorption combines with the molecular size effects on diffusion, to cause permeation to not be monotonic with molecular weight. Other interaction effects due to pH and the presence of co-ions have been observed. Limited mixture studies indicate separation factors slightly higher than those predicted by pure component permeation are obtained. It was also found that films which are initially impermeable to YADH may be made gel-like and thus YADH-permeable by con-trolled treatment with glutaraldehyde crosslinking.

101,284 PB91-174565 Not available NTIS National Inst. of Standards and Technology (NML), Gathersburg, MD. Organic Analytical Research Div. Planar Waveguide Optical Immunosensors.

Final rept.

S. J. Choquette, L. Locascio-Brown, and R. A. Durst. 1990, 6p
Pub. in Proceedings of SPIE (Society of Photo-Optical Instrumentation Engineers) Chemical, Biochemical, and Environmental Fiber Sensors II, San Jose, CA., September 19-21, 1990, v1368 p258-263.

Keywords: \*Theophylline, Monoclonal antibodies, Fluorescence, Liposomes, Reprints, \*Planar waveguides, Immunosensors.

Monoclonal antibodies were covalently bonded to the surfaces of planar waveguides to confer immunoreac-

## MEDICINE & BIOLOGY

# Biochemistry

tivity. Silver-ion diffused waveguides were used to measure theophylline concentrations in a fluorescence immunoassay, and silicon nitride waveguides were used to detect theophylline in an absorbance-based immunoassay. Liposomes were employed in both assays as the optically detectable label in a competitive reaction to monitor antigen-antibody complexation. Regeneration of the active antibody site will be discussed

101,285

PB91-175349 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Chemical Thermodynamics Div. Neutron Crystallography of Proteins.

Final rept.

N. V. Raghavan, and A. Wlodawer. 1987, 31p Pub. in Methods of Experimental Physics, v23 ptC p335-365 1987.

Keywords: \*Single crystals, \*Neutron diffraction, \*Proteins, \*Biochemistry, Crystal structure, Solvents, Solvolysis, Hydrogen isotopes, Labeled reactions, Isotope exchange, Reprints.

Single crystal neutron diffraction has reached the stage where the efforts of the last fifteen years are beginning to provide results. Three facilities are now available for data collection. Although large crystals are still desirable, their sizes no longer limit successful neutron analyses. The results of hydrogen exchange experiments and of methyl rotor analyses provide unique methods for correlating the dynamic properties of proteins with their three-dimensional structures. Such motions in proteins are thought to play an important role in their function and may affect processes such as ligand binding, enzyme catalysis, and electron transfer. Finally, the improved description of the bound solvent that is obtained by neutron diffraction and the differentiation of solvent components is also gaining in importance.

101,286

PB91-189472 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Ionizing Radiation Div. 8-Hydroxyguanine Content of Isolated Mitochondria Increases with Lipid Peroxidation.

Final rept. A. M. Hruszkewycz, and D. S. Bergtold. 1990, 6p Pub. in Mutation Research 244, n2 p123-128 1990.

Keywords: \*Lipid peroxidation, \*Mitochondria, Alphatocopherol, Deoxyribonucleic acids, DNA damage, Agar gel electrophoresis, Reprints, \*8-hydroxyguan-

When lipid peroxidation was induced in isolated mitochondria there was a marked increase in the 8-hydroxyguanine content of the nucleic acids extracted from these mitochondria. The elevation of 8-hydroxyguan-ine levels was associated with an extensive alteration of normal electrophoretic mobility of mitochondrial DNA. However, suppression of lipid peroxidation with alpha-tocopherol proportionally attenuated 8-hydroxyguanine production and limited the electrophoretic mobility change of mitochondrial DNA.

101,287

PB91-189886
Not available NTIS
National Inst. of Standards and Technology (NML),
Boulder, CO. Chemical Engineering Science Div.
Enhanced Transport and Liquid Membranes in Bioseparations.

Final rept.

J. Pellegrino, and R. Noble. 1990, 9p Pub. in Trends in Biotechnology 8, p216-224 Aug 90.

Keywords: \*Biological transport, \*Chemical reactions, \*Artificial membranes, Reprints, \*Bioseparations.

Membranes that use a reversible chemical reaction or sequestration to achieve high selectivities and producivities show great potential for use in bioseparations was studied. The concept of liquid membranes, with and without a complexing agent (carrier), and the types of system configurations and carriers that may be used with these membranes, are discussed.

101.288

PB91-194803 Not available NTIS National Inst. of Standards and Technology (CSTL), Gaithersburg, MD. Biotechnology Div.

Thermodynamics of Hydrolysis of Oligosaccharides.

Final rept.

R. N. Goldberg, D. Bell, Y. B. Tewari, and M. A. McLaughlin. 1991, 8p

Pub. in Biophysical Chemistry 40, p69-76 1991.

Keywords: \*Thermodynamics, \*Oligosaccharides, Hydrolysis, Enthalpy, High pressure liquid chromatography, Chemical reactions, 1,4-alpha-glucosidase, Reprints, Beta-fructofuranosidase,

Microcalorimetry has been used to determine enthalpy changes for the hydrolysis of a series of oligosaccarides. High-pressure liquid chromatography was used to determine the extents of reaction and to check for any possible side reactions. The enzyme glucan 1,4-alpha-glucosidase was used to bring about the following hydrolysis reactions: (A) maltose(aq) + H2O(liq) = 3D-glucose(aq); (B) maltotriose(aq) + 2H2O(liq) = 3D-glucose(aq); (C) maltotetraose(aq) + 3H2O(liq) = 4D-glucose(aq); (D) maltopentaose(aq) + 4H2O(liq) = 5D-glucose(aq); (F) maltohexaose(aq) + 5H2O(liq) = 6D-glucose(aq); (G) amylose(aq) + nH2O(liq) = (n+1) D-glucose(aq); (G) amylose(aq) + 2H2O(liq) = 3D-glucose(aq); (J) isomaltotriose(aq) + 2H2O(liq) = 3D-glucose(aq). The enzyme beta-fructofuranosidase was used for the reactions; (K) raffinose(aq) + H2O(liq) = ides. High-pressure liquid chromatography was used glucose(aq). The enzyme beta-fructofuranosidase was used for the reactions; (K) raffinose(aq) + H2O(liq) = alpha-D-melibiose(aq) + D-fructose(aq); and (L) stachyose(aq) + H2O(liq) = o-alpha-D-galactopyranosyl-(1 -> 5)-alpha-D-galactopyranosyl-(1 -> 6)-alpha-D-glucopyranose + D-fructose(aq). These processes correspond to the hydrolysis of the following linkages: glucose-glucose (alpha, 1 -> 4) glucose-glucose (alpha, 1 -> 6), and glucose-fructose (1 -> 6). The respective enthalpy changes accompanying the hydrolysis of these linkages are -453, 5.8 and -15.0 k1/mol. Both these results and available thermodykJ/mol. Both these results and available thermody-namic data in the literature demonstrate that additivity works well in predicting the thermodynamics of hydrolysis reactions involving oligosaccharides.

101,289

PB91-195701 Not available NTIS

Not available NTIS
National Inst. of Standards and Technology (CSTL),
Gaithersburg, MD. Biotechnology Div.
Thermodynamics of Hydrolysis of Disaccharides:
Lactulose, alpha-D - Melibiose, Palatinose, D - Turanose and 3-o-beta-D-Galactopyranosyl-D-arabinose.
Final rest

Final rept.

Y. B. Tewari, and R. N. Goldberg. 1991, 9p See also PB89-186761.

Pub. in Biophysical Chemistry 40, p59-67 1991.

Keywords: \*Thermodynamics, \*Disaccharides, Hydrolysis, High pressure liquid chromatography, Enthalpy, Entropy, Beta-galactosidases, Fructose, Galactose, Sucrose, Glucose, Reprints.

High-pressure liquid chromatography and microcalorimetry have been used to study the thermodynamics of the hydrolysis reactions of a series of dissaccharides. The enzymes used to bring about the hydrolyses were beta-galactosidase for lactulose and 3-o-beta-D-galactosidase for lactulose and 3-o-beta-D-galactosidase. topyranosyl-D-arabinose; beta-glucosidase for alpha-D-melibiose; beta-amylase for D-trehalose; isomaltase for platinose; and alpha-glucosidase for D-turanose. The buffer used was sodium acetate (0.02-0.10 M and pH 4.44-5.65). These six processes correspond, respectively, to the hydrolysis of the following linkages: galactose-fructose (1 -> 4), galactose-glucose (1 -> 6), glucose-fructose (1 -> 6), glucose-fructose (1 -> 3), and galactose-ambinations of the following linkages: ose (1 -> 3). Using available data in the literature, the heat capacity changes for these processes are found to be in the range - 36 to - 69 J/mol/K. The available thermodynamic data on the hydrolysis of disaccharides is summarized. It is found that the entropy changes for the hydrolysis of disaccharides are in the range 31 - 56 J/mol/K and are well represented by an average value of 40 + or - 7 J/mol/K. The abnormally high enthalpy of hydrolysis of aqueous sucrose (-14.96 kJ/mol) can be explained by consideration of the enthalpy of conversion of fructopyranose to fructofuran-

101.290

Not available NTIS PB92-116953 National Inst. of Standards and Technology (NML), Gaithersburg, MD. Ionizing Radiation Div.

Formation of ortho-Tyrosine by Radiation and Organic Solvents in Chicken Tissue. Final rept.

L. R. Karam, and M. G. Simic. 1990, 5p Pub. in Jnl. of Biological Chemistry 265, n20 p11581-11585, 15 Jul 90.

Keywords: \*Poultry, \*Tyrosine, \*Organic solvents, \*Radiation, Tissues(Biology), Mass fragmentography, Dose-response relationships, Reprints

Fresh chicken breast and beef incubated in water were found to contain no o-Tyr at the current levels of detection (0.1 ppm) by capillary gas chromatography/mass spectrometry and selective ion monitoring. In contrast, samples incubated at 37 C in the presence of ethanol, samples incubated at 37 C in the presence of ethanol, benzene, or carbon tetrachloride (used in fat extraction) contained large quantities (2.5-5.1 ppm) of o-Tyr. No o-Tyr was detected in the water-insoluble fraction of meat treated with carbon tetrachloride after triple extraction by water. However, reaction of radiation generated OH in gamma-irradiated fresh chicken tissue with endogenous phenylalanine yields o-Tyr with a linear yield-dose response in both water-soluble and insoluble tissue fractions and -insoluble tissue fractions.

# Clinical Chemistry

101,291

PB91-147629 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Organic Analytical Research Div. Liposome Flow Injection Immunoassay: Implica-tions for Sensitivity, Dynamic Range, and Antibody Regeneration. Final rept.

L. Locascio-Brown, A. L. Plant, V. Horvath, and R. A. Durst. 1990, 7p Pub. in Analytical Chemistry 62, n23 p2587-2593, 1

Keywords: \*Liposomes, \*Immunoassay, \*Theophylline, Antibodies, \*Flow injection analysis.

The report describes the use of a liposome-based flow The report describes the use of a hiposome-based now injection immunoassay (FIIA) system for quantitation of a clinical analyte, theophylline. With very minor changes in assay format, the procedure can also be used for the quantitation of anti-theophylline. Automated sequential analyses were performed at room temperature with picomole sensitivity and a day-to-day co-efficient of variation of less than 5% for aqueous solu-tions. The system components include liposomes that contain fluorophores in their aqueous centers and an immobilized-antibody reactor column. The immunoreactor was regenerated hundreds of times over 3 months of continuous use with no measurable loss of antibody activity. The two assay formats studied produced distinct dynamic ranges for their respective analytes. The special advantages of using flow injection analysis for immunoassays and of using liposomes in FIIA are discussed.

101,292

PB91-189266 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Organic Analytical Research Div. Stability of Uric Acid in Ammonium Hydroxide.

P. Ellerbe, A. Cohen, M. J. Welch, and E. White V. Pub. in Clinical Chemistry 34, n11 p2280-2282 1988.

Keywords: \*Uric acid, \*Stability, \*Ammonia, Decomposition reactions, Chemical analysis, Mass spectroscopy, Allantoin, Urea, Reprints.

The stability of uric acid in dilute aqueous ammonium hydroxide solution was examined by mass spectrometry. Uric acid decomposes in ammonium hydroxide even at the low concentration of 0.015 M at a mole ratio of ammonium hydroxide to uric acid of 50:1. The slope of the decomposition curve indicates that uric acid was being destroyed at an initial rate of several percent per hour. There are at least four products of the decomposition two of which have been identified as allantoin and urea. Uric acid does not detectably decompose in ammonium hydroxide at a concentration of 0.001 M and mole ratio of ammonium hydroxide to uric acid of 3.4 or less. The results have certain implications. Firstly, any method for the determination of

# **Clinical Chemistry**

uric acid that involves treating the analyte with ammonium hydroxide before analysis may destroy it. Secondly, a published 'definitive' method for uric acid could produce incorrect results because the uric acid is stored in 0.015 M ammonium hydroxide at a mole ratio oif over 120:1 of ammonium hydroxide to uric

Clinical Medicine

101 293 PB91-195198 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Ionizing Radiation Div.
Intensifying Effect of Metallic Screens on the Sensitivity of X-ray Films for 400-kV Bremsstrahlung

Photons.

Final rept.

101,294

E. Navon, C. E. Dick, and G. Barnea. 1991, 6p Pub. in Medical Physics 18, n2 p299-304 Mar/Apr 91.

Keywords: \*Radiographic films, \*X ray film, \*Radiation effects, \*Electron bombardment, Bremsstrahlung, Lead(Metal), Aluminum, Copper, Foils(Materials), Sensitivity, Reprints, Metal screens, Intensification factors.

Measurements are carried out to determine the relative photographic effect produced by electrons ema-nating from metallic screens on a typical radiographic film. The electrons are produced in metal foils of aluminum, copper, and lead by the interaction of photons in a 400-kV bremsstrahlung beam. Intensification factors of up to 1.65, 2.05, and 5.90 for aluminum, copper, and lead screens, respectively, are determined as a function of the foil thickness. The equilibrium thickness screens are determined to be 20 mg/sq cm for aluminum and 30 mg/sq cm for copper and lead. These results are compared with the absorbed dose in the film emulsions, calculated by Monte Carlo methods. The results of the present work are compared with those for (60)Co and (137)Cs photon beams. The dependence of the equilibrium thickness and the intensifica-tion factor on photon energy and the atomic number of the screen material is summarized and explained.

PB91-203745 Not available NTIS National Bureau of Standards (IMSE), Gaithersburg, MD. Metallurgy Div. Mossbauer Imaging. Final rept. S. J. Norton. 1988, 1p See also PB89-176895. Pub. in Physics Bulletin 39, n5 p182 1988.

Keywords: \*Mossbauer effect, \*Imaging techniques, \*Computerized tomography, \*Spectroscopy, Metallography, Diagnostic techniques, Tests, Reprints.

Imaging techniques are playing an increasingly impor-tant role in many areas of research. Although NMR has long been employed as an important spectroscopic tool in chemistry, biology and materials science, a significant recent advance is nuclear-magnetic-reso-nance (NMR) imaging. Now the Mossbauer effect, an-other well-established spectroscopic technique, has also been proposed as the basis of a new imaging method (S. J. Norton, Nature, 12 Nov., 1987).

101.295 PB92-116623 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Statistical Engineering Div.
Use of Cross-Validation as a Stopping Rule in
Emission Tomography Image Reconstruction. Final rept.

Pub. in Proceedings of SPIE (Society of Photo-Optical Instrumentation Engineers) - Medical Imaging V: Image Physics, v1443 p226-233 1991.

Keywords: \*Image reconstruction, \*Tomography, Stopping rules(Mathematics), Reprints, \*Positron emission tomography, EM algorithm, Cross validation.

Simulated and real Positron Emission Tomography (PET) images are reconstructed using the iterative EM algorithm. The data is split up into independent parts. The EM algorithm is applied to each part and stopped according to a cross-validation procedure. For a variety of simulated and real data sets, stopping points

were reached. For simulated data, the average of the reconstructions from a four-way split of the data was visually superior to the reconstruction obtained by applying the EM algorithm to the full data and stopping at a subjectively chosen iteration. For real data, such an improvement was not observed. To remove point artifacts, the reconstructions were filtered.

101,296 PB92-117142 Not available NTIS Notional Inst. of Standards and Technology (NML), Saithersburg, MD. Ionizing Radiation Div. Photon Energy Dependence of the Sensitivity of Radiochromic Film and Comparison with Silver Halide Film and LiF TLDs Used for Brachytherapy Dosimetry.

Final rept. P. J. Muench, A. S. Meigooni, R. Nath, and W. L. McLaughlin. 1991, 7p Sponsored by Public Health Service, Rockville, MD.

Pub. in Medical Physics 18, n4 p769-775 Jul/Aug 91.

Keywords: \*Brachytherapy, \*Film dosimetry, \*Ther-moluminescent dosimetry, \*Photons, Comparison, Iridium, Silver halides, Ionizing radiation, Polymeriza-tion, Dyes, Reprints, \*Radiochromic film.

There is a new radiochromic film, a highly uniform, thin (100 micrometers) etector whose sinsitive layer (6 micrometers thick) changes from colorless to blue by dye polymerization without processing, upon exposure to ionizing radiation. Because the dose gradients around brachytherapy sources are steep, the high spatial res-olution offered by film dosimetry is an advantage over other detectors such as thermoluminescent dosimeters (TLDs). This compares the photon energy de-pendence of the sensitivities of GafChromic film, silver halide verification film (Kodak X-Omat V Film), and lithium fluoride TLDs (Harshaw), over the photon energy range 28 keV to 1.7 MeV, which is of interest in bra-chytherapy. Sensitivity of the radiochromic film is ob-served to decrease by about 30% as effective photon energy decreases from 1710 keV (4-MV x rays) to 28 keV (60-kV x rays, 2-mm Al filter). In contrast, the sensitivity of verification film increases by 980% and that of LiF TLDs increases by 41%. Radiochromic film, like LIF TLDs, does not exhibit the drastic sensitivity changes below 127 keV that silver halide film exhibits. Dose distribution in the immediate vicinity of a high activity (370 GBq) brachytherapy (192) Ir source has been mapped using radiochromic film and is presented to illustrate the applicability of this new technology to brachytherapy dosimetry.

### Cytology, Genetics, & Molecular Biology

PB91-134767 Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Chemical Engineering Science Div. Gravity-Dependent Phenomena at the Scale of the Single Cell.

Final rept. P. Todd. 1989, 19p Pub. in American Society for Gravitational and Space Biology Bulletin 2, p95-113 Aug 89.

Keywords: \*Cells(Biology), Reduced gravity, Sedimentation, Diffusion, Solutes, Gravity, Reprints, Gravitational effects, Intracellular transport, Convective flow.

Progress in gravitational cell biology research will depend on the continuing evaluation of a wide variety of physical phenomena affected by gravity and their roles in extracellular, intercellular, and intracellular processes. The paper examines those responses of organisms to gravity which depend on functions at the single cell level. Single cell functions are affected by perturbations in their internal and external environment by a variety of factors, one of which is the effect of gravity. In a microgravity environment extracellular solutes must be transported by diffusion or active circulatory processes in the absence of density gradientdriven convection, and flocculation and coalescence are reduced by the lack of motion of aggregates.

Not available NTIS PB91-148098 National Bureau of Standards (NML), Gaithersburg, MD. Chemical Thermodynamics Div.

Multiple Conformations of Amino Acid Residues in Ribonuclease A.

Final rept.

L. A. Svensson, L. Sjolin, G. L. Gilliland, B. C. Finzel, and A. Wlodawer. 1986, 6p

Pub. in Proteins: Struct., Funct., Genet. 1, n4 p370-375

Keywords: \*Amino acids, \*Pancreatic ribonuclease, \*Protein conformation, Structure-activity relationship, Protein engineering, Reprints.

Highly refined 1.26A structure (R = 0.15) of phosphate-free bovine pancreatic ribonuclease A was modeled with 13 residues having discrete multiple conformations of side chains. These residues are widely distributed over the protein surface, but only one of them Lys 61, is involved in crystal packing interactions. The discrete conformers have no unusual torsion angles and their interactions with the solvent and with other atoms of the protein are similar to those residues modeled with a single conformation. For three of the residues, Val 43, Asp 83, and Arg 85, two correlated conformations are found. The observed plasticity in the protein surface will be of significance in analyzing structure - function relationships and in performing protein engineering.

101.299

PB91-148213 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Chemical Thermodynamics Div.

Crystallizing Catabolite Gene Activator Protein with cAMP for Structural Analysis.

Final rept.

I. T. Weber, 1988, 8p

Pub. in Methods in Enzymology 159, p278-285 1988.

Keywords: \*Adenosine cyclic monophosphate, \*Catabolite gene activator proteins, Binding sites, Protein kinases, Protein conformation, DNA-binding proteins, Regulator genes, Reprints.

The crystal structure of the CAP dimer with cAMP has provided many insights into the action of this gene regulatory protein. The CAP subunit is divided into two domains that are connected by a hinge region. The car-boxy-terminal domains bind to DNA and show both se-quence and structural homologies with many other gene regulatory proteins from bacteria and viruses. The amino-terminal domain forms a binding site for cAMP and has been used to model the cAMP-binding domains of the regulatory subunits of mammalian cAMP-dependent protein kinase.

101,300

PB91-149229 Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Chemical Engineering Science Div. Hydrodynamics and Mass Transfer in Two-Phase Aqueous Extraction Using Spray Columns. Final rept.

S. B. Sawant, S. K. Sikdar, and J. B. Joshi. 1990, 7p Pub. in Biotechnology and Bioengineering 36, p109-115 1990.

Keywords: \*Hydrodynamics, \*Mass transfer, \*Sprays, \*Albumins, \*Separation, Polyoxyethylene, Dextran, Phase velocity, Reprints, \*Two phase aqueous extrac-

Spray columns can be used to isolate and purify proteins using the two-phase aqueous extraction technique based on polyethylene glycol (PEG) and dextran. The fractional dispersed phase (PEG) holdup and overall mass transfer coefficients were measured in a 9.7 mm i.d. spray column. The authors found that the dispersed phase holdup increased with increasing PEG phase velocity. The overall mass transfer coefficients for bovine serum albumin, normalized for the PEG holdup, were found to be independent of the PEG phase velocity. The result was expected, since true mass transfer coefficients do not vary with phase ve-

101.301

PR91-175604 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Chemical Thermodynamics Div.

### **MEDICINE & BIOLOGY**

# Cytology, Genetics, & Molecular Biology

Crystal Structure of Phosphate-Free Ribonucle-

Final rept. A. Wlodawer, G. I. Gilliland, L. Sjolin, and L. A. Svensson. 1987, 10p Pub. in UCLA (University of California, Los Angeles)

Symposium on Molecular and Cellular Biology 69, n2 p109-118 1987.

Keywords: \*Ribonucleases, \*Crystal structure, \*Protein conformation, Pancreas, Amino acids, Phosphates, Binding sites, Butanols, Molecular models, Re-

The crystal structure of phosphate-free bovine pancreatic ribonuclease has been refined with 1.26 A resolu-tion X-ray diffraction data. The final R factor was 15%, with the rms deviation of bond lengths from ideality of 0.024 A. Even in the absence of the anion bound in the active site, only minor movements of the side chains were noticed in that area. Thirteen amino acids, all but one of them on the protein surface, were modeled with two different conformations of the side chains. The bound solvent of the refined model includes a t-butanol and 188 fully or partially occupied water sites. The structure was compared in detail with three other highly refined models of ribonuclease.

Not available NTIS PB91-187476 National Inst. of Standards and Technology (CSTL), Gaithersburg, MD. Biotechnology Div. 46Gas Chromatography-Mass Spectrometry of

Free Radical-Induced Products of Pyrimidines and Purines in DNA.

Final rept.

M. Dizdaroglu. 1990, 16p Pub. in Methods of Enzymology 193, p842-857 1990.

Keywords: \*Deoxyribonucleic acids, \*Pyrimidines, \*Purines, \*DNA damage, \*Free radicals, Mass fragmentography, Hydrolysis, pH, Reprints.

A description is provided of the application of the gas chromatography-mass spectrometry (GC-MS) technique to measurement of products of pyrimidines and purines in DNA, which are formed by reactions of free radicals with DNA. Acidic or enzymatic hydrolyses are used to free base products as bases or nucleosides prior to their analysis by GC-MS. Acidic hydrolysis re-leases DNA base-amino acid crosslinks from nucleoprotein. The trimethylsilyl derivatives of all these products provide characteristic mass spectra, which contain a molecular ion and other typical ions of this class of compounds. The tbutyldimethylsilyl derivatives are also used for measurement of modified bases. The use of the selected-ion monitoring technique permits the characterization and quantitative measurement of the products at low concentrations. Examples of mass spectra are presented and the fragmentation patterns of the molecules are discussed.

101,303 PB91-187484 Not available NTIS National Inst. of Standards and Technology (CSTL),

Gaithersburg, MD. Biotechnology Div.

Measurement of DNA Base Damage and DNA-Protein Cross-Links in Mammalian Chromatin. Final rept.

M. Dizdaroglu. 1990, 14p Sponsored by Department of Energy, Washington, DC. Pub. in lonizing Radiation Damage to DNA: Molecular Aspects, p17-30 1990.

Keywords: \*DNA damage, \*DNA-binding proteins, \*Chromatin, Ionizing radiation, Cross-linking reagents, Mass fragmentography, Mammals, Free radicals, Re-

Methodologies incorporating the technique of gas chromatography/mass spectrometry (GC/MS) have been developed in recent years for measurement of DNA damage produced by ionizing radiation or by other free radical-generating systems. GC/MS with selected-ion monitoring (SIM) facilitates unequivocal identification and quantitation of a plethora of products of all four bases in DNA. In addition, DNA-protein cross-links in mammalian chromatin are unequivocally identified and quantitated. The sensitivity and selectivity of the GC/MS-SIM technique also enables the measurement of DNA base products in isolated mammalian chromatin without the necessity of first isolating DNA. Recent results demonstrate the usefulness of the GC/MS technique for measurement of DNA damage in DNA as well as in mammalian chromatin under a vast variety of conditions of free radical pro101,304

PB91-189365 Not available NTIS National Inst. of Standards and Technology (CSTL), Gaithersburg, MD. Biotechnology Div. Hydroxyl Radical Induced Cross-Linking of Cytosine and Tyrosine in Nucleohistone.

Final rept.

E. Gajewski, and M. Dizdaroglu. 1990, 4p Pub. in Biochemistry 29, n4 p977-980 1990.

Keywords: \*Cytosine, \*Tyrosine, \*Hydroxyl radicals, Cross-linking reagents, Mass fragmentography, Gamma rays, Hydrolysis, Reprints, \*Nucleohistones.

Hydroxyl radical induced formation of a DNA-protein cross-link involving cytosine and tyrosine in nucleohistone in buffered aqueous solution is reported. The technique of gas chromatography-mass spectrometry was used for the investigation. A gamma-irradiated aqueous mixture of cytosine and tyrosine was first investigated in order to obtain gas chromatographic-mass spectrometric properties of possible cytosine-ty-rosine cross-links. One cross-link was observed, and its structure was identified as the product from the for-mation of a covalent bond between carbon 6 of cytosine and carbon 3 of tyrosine. With the use of gas chromatography-mass spectrometry with selected-ion monitoring, this cytosine-tyrosine cross-link was identified in acidic hydrolysates of calf thymus nucleohistone gamma-irradiated in N2O-saturated aqueous solution. The yield of the DNA-protein cross-link in nucleohistone was found to be a linear function of the radi ation dose in the range of 100-500 Gy (J/kg). The yield amounted to 0.05 nmol/J. Mechanisms uderlying the formation of the cytosine-tyrosine cross-link in nucleohistone were proposed to involve radical-radical and/ or radical addition reactions of hydroxyl adduct radicals of cytosine and tyrosine moieties, forming a covalent bond between carbon 6 of cytosine and carbon 3 of tyrosine. When oxygen was present in irradiated solutions, no cytosine-tyrosine cross-links were observed.

101.305

PB91-190074 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Chemical Thermodynamics Div. Crystal Structure of a cAMP-Independent Form of Catabolite Gene Activator Protein with Adenosine Substituted in One of 2 cAMP-Binding Sites. Final rept.

M. C. Vaney, G. L. Gilliland, J. G. Harman, A. Peterkofsky, and I. T. Weber. 1989, 7p Pub. in Biochemistry 28, n11 p4568-4574 1989.

Keywords: \*Catabolite gene activator proteins, \*Adenosine cyclic monophosphate, \*Crystallization, \*Protein conformation, \*Adenosine, Binding sites, Genetic transcription, Operon, Escherichia coli, Mutation, X-ray diffraction, Reprints.

Catabolite gene activator protein (CAP) in the presence of cAMP stimulated transcription from several operons in E. coli. A cAMP-independent variant, in which Ala144 is replaced by Thr (CAP91), has been crystallized as the cAMP complex. CAP91, unlike the wild-type CAP, is activated by analogs of cAMP, including adenosine. In order to test the effect of adenosine on the structure, a crystal of CAP91 was soaked in a solution of 10mM adenosine, and X-ray diffraction data solution of 10mM adenosine, and X-ray diffraction data were measured to 3.5 A resolution. The difference Fourier map calculated with phases from the CAP91 structure showed significant negative density at the position of the phosphate of cAMP bound in the 'closed' subunit of the CAP91 dimer. This was consistent with the replacement of adenosine for cAMP in the 'closed' subunit. The cAMP-binding site of the 'open' subunit was apparently still occupied by cAMP. The coordinates were refined by restrained least-square to an B factor of 20.2% Adenosine is bound in the an R factor of 20.2%. Adenosine is bound in the cAMP-binding pocket in almost the same position as cAMP, however, the new position of 5'OH of adenosine allowed formation of two new hydrogen bonds with Ser 83, instead of the interactions of the phosphate of cAMP with Arg 82 and Ser 83.

101.306

PB91-200824 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Chemical Kinetics Div.

Iron Ion-Dependent Modification of Bases in DNA by the Superoxide Radical-Generating System Hypoxanthine/Xanthine Oxidase.

O. I. Aruoma, B. Halliwell, and M. Dizdaroglu. 1989,

Pub. in Jnl. of Biological Chemistry 264, n22 p13024-13028, 5 Aug 89.

Keywords: \*Deoxyribonucleic acids, \*Superoxide, \*Hypoxanthines, \*Xanthine oxidase, \*Iron, Mass fragmentography, Hydroxyl radicals, DNA damage, Hydrolysis, lons, Reprints.

Damage to the bases in DNA produced by the hypoxanthine/xanthine oxidase system in the presence of iron ions was studied. The base products in DNA were iron ions was studied. The base products in DNA were measured using gas chromatography-mass spectrometry with selected ion monitoring after acidic hydrolysis of DNA and trimethylsilylation. Products identified were cytosine glycol, thymine glycol, 5,6-dihydroxycytosine, 4,6-diamino-5-formamidopyrimidine, 8-hydroxyyadenine, 2,6-diamino-4-hydroxy-5-formamidopyrimidine, and 8-hydroxyguanine. These are typical hydroxyl cytosine, 4,6-diamino-5-formamidopyrimidine, 5,6-dihydroxycytosine, 4,6-diamino-5-formamidopyrimidine, 5,6-dihydroxycyt and 8-hydroxyguanine were proposed as the products in DNA to measure if one aims to measure DNA products as indices of oxidative DNA damage involving hydroxyl radicals in vivo.

101,307

PB91-202960 Not available NTIS
National Inst. of Standards and Technology (NML),
Gaithersburg, MD. Chemical Kinetics Div.
Selected-Ion Mass Spectrometry: Assays of Oxidative DNA Damage. Final rept.

M. Dizdaroglu, and E. Gajewski. 1990, 15p Pub. in Methods in Enzymology 186, p530-544 1990.

Keywords: \*Mass spectrometry, \*Oxidation, \*DNA damage, lons, Mass fragmentrography, Hydrolysis, Hydroxyl radicals, Cross-linking reagents, Nucleoproteins, DNA-binding proteins, Reprints.

Chemical characterization and quantitative measurement of oxidative damage to DNA caused by free radicals is essential for an understanding of the biological consequences of such damage. The present article describes the technical details of the application of the gas chromatography-mass spectrometry (GC-MS) technique to measurement of DNA damage caused by hydroxyl radicals. Reactions of hydroxyl radicals form a variety of base products in DNA and DNA-protein crosslinks in nucleoprotein. Acidic or enzymatic hydrocrosslinks in nucleoprotein. Acidic or enzymatic hydro-yses are used to free base products as bases or nu-cleosides prior to their analysis by GC-MS. Acidic hy-drolysis releases DNA base-amino acid crosslinks from nucleoprotein. The trimethylsily derivatives of all these products provide characteristic mass spectra, which contain a molecular ion and other typical ions of this class of compounds. The use of the selected-ion monitoring technique permits the characterization and quantitative measurement of the products at low con-centrations centrations.

101.308

PB91-237198 Not available NTIS National Inst. of Standards and Technology (CSTL), Gaithersburg, MD. Biotechnology Div.

Immobilization of Binding Proteins on Nonporous Supports Comparison of Protein Loading, Activity, and Stability.

Final rept. A. L. Plant, L. Locascio-Brown, W. Haller, and R. A. Durst. 1991, 16p

Pub. in Applied Biochemistry and Biotechnology 30, p83-98 1991.

Keywords: \*Proteins, \*Binding sites, \*Glass, \*Nylon, \*Polystyrene, Monoclonal antibodies, Theophylline, Biotin, Ligands, Radioactivity, Reprints.

Four different nonporous particulate materials, nylon, polystyrene, soda-lime silicate glass, and fused silica glass, have been evaluated for their appropriateness as immobilization supports for immunoglobulins. A method of protein quantitation that is usually applied to solutions, the bicinchoninic acid (BCA) assay, was used successfully to directly measure ng amounts of protein immobilized on the supports. Two proteins, a monoclonal antibody to theophylline and the biotin binding protein avidin, were studied. Radioactive theo-

# Cytology, Genetics, & Molecular Biology

phylline and radioactive biotin were used to measure the activity of the immobilized protein. Ligand binding capacity per sqmm of support was measured as a function of amount of protein immobilized. The binding activity of biotinyl-antibody conjugate immobilized on avidin-adsorbed polystyrene is stable, even when stored for over 22 wk. Antibody covalently immobilized on soda-lime silicate glass beads retains its binding.

101,309 PB91-237362 Not available NTIS National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Reactor Radiation Div. Ab Initio Phase Determination for X-ray Diffraction Data from Crystals of a Native Protein. Final rept. L. Sjolin, E. Prince, L. Anders Svensson, and G. L. Gilliland. 1991, 8p

Pub. in Acta Crystallographica A47, p216-223 1991.

Keywords: \*Proteins, \*Crystal structure, \*Phase diagrams, Algorithms, X ray diffraction, Fourier transformation, Electron density, Molecular structure, Cattle, Reflection, Entropy, Reprints, \*Bovine chymosin.

An efficient algorithm for the determination of an everywhere positive electron-density distribution that agrees with observed structure amplitudes has been used to determine the phases of X-ray diffraction data from recombinant bovine chymosin, a protein with 323 amino-acid residues in the molecular chain whose structure was recently determined using molecular re-placement methods. A systematic procedure for test-ing the signs of centric reflections, using the total en-tropy of the map as a figure of merit, was used to produce a low-resolution map. The phases of acentric and additional centric reflections were then chosen by adding them to the map with various possible phases and computing the total entropy of the resulting map. The molecule is many times larger than any whose structures have previously been determined without the use of isomorphous replacement, molecular replacement or anomalous dispersion, and the map demonstrates the potential of maximum-entropy methods in macromolecular structure determination.

PB91-237560 Not available NTIS National Bureau of Standards (NEL), Boulder, CO. Not available NTIS Chemical Engineering Science Div. Low-Cost Aqueous Two-Pha Two-Phase System for Enzyme Extraction.

Final rept.

D. C. Szlag, and K. A. Giuliano. 1988, 6p Pub. in Biotechnol. Tech. 2, n4 p277-282 1988.

Keywords: \*Enzymes, \*Extraction, Purification, Alcohol dehydrogenase, Polyoxyethylene, Dextran, Separation, Viscosity, Yeasts, Reprints, Maltodextrins.

Several low-cost maltodextrins formed two liquid phases with polyethylene glycol (PEG) in aqueous solution. The physical characteristics of these maltodextrin/PEG systems are similar in many respects to dextran/PEG systems except for the cost. Maltodextrins are currently available for \$0.56/kg as compared to \$150/kg for fractionated dextran (industrial grade). The remarkable cost savings makes the large scale application of polymer-polymer aqueous two-phase extractions commercially viable. The authors have measured some of the physical properties of the maltodextrin/PEG two-phase systems and found them to exhibit low viscosities and excellent processibility. Extraction of alcohol dehydrogenase from homogenized yeast cells and yeast enzyme concentrate was per-formed in both PEG/dextran and PEG/maltodextrin systems using PEG bound Cibacron blue. Greater purification factors were measured for the PEG/maltodextrin system for similar recoveries.

101,311 PB91-237602 Not available NTIS National Inst. of Standards and Technology (CSTL), Gaithersburg, MD. Biotechnology Div. Thermodynamics of Industrially Important

Enzyme Catalyzed Reactions.

Final rept. Y. B. Tewari. 1990, 17p Pub. in Appl. Biochem. Biotechnol. 23, n3 p187-203 1990

Keywords: \*Thermodynamics, \*Enzymes, \*Catalysis, Penicillins, Chemical reactions, Amino acids, Saccharides, Enthalpy, Reprints.

The paper presents an examination of the thermodynamics of ten industrially important enzyme catalyzed reactions. The reactions discussed are: the conversions of penicillin G to 6-amino-penicillinic acid using the enzyme penicillin acylase; starch to glucose using amylases; glucose to fructose using glucose (xylose) isomerase; cellulose to glucose using cellulase; fumaric acid and ammonia to L-aspartic acid using L-aspartase; transcinnamic acid and ammonia to L-phenylalanine using L-phenylalanine ammonia-lyase: L-histidine to urocanic acid and ammonia using L-histidine ammonia-lyase; lactose to glucose and galactose using lactase; and the reactions catalyzed by aminoacylases and proteases. The selection of these processes was based on the economic value of the products and their intrinsic industrial importance. The available thermodynamic properties, such as equilibrium constants, Gibbs energies (Delta G), enthalpies (Delta H), and heat capacity changes (Delta C(sub p)) of these enzyme catalyzed reactions are reviewed and summarized. Recommendations are made for future research in this area.

101,312 PB92-116912 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Chemical Thermodynamics Div. Damage to the Bases in DNA Induced by Stimulated Human Neutrophils. Final rept.

J. H. Jackson, P. A. Hyslop, I. U. Schraufstatter, C. G. Cochrane, M. Dizdaroglu, A. F. Fuciarelli, and E. Gajewski. 1989, 6p Pub. in Jnl. of Clinical Investigation 84, n5 p1644-1649

Keywords: \*DNA damage, \*Neutrophils, Free radicals, Mass fragmentography, Carcinogens, Base pairs, Thymus gland, Reprints.

Inflammatory leukocytes (neutrophils) have been associated with carcinogenesis in chronic inflammation and malignant transformation of cells. Stimulated neutrophils have been known to cause DNA damage. Here, the authors report on the chemical characterization of base damage in DNA induced by a tumor promotor-stimulated human neutrophils. Calf thymus DNA was treated with stimulated neutrophils in the presence and absence of iron ions, and then analyzed by gas chromatography-mass spectrometry with selected-ion monitoring. Cytosine glycol, thymine glycol, 4,6-diamino-5-formamidopyrimidine, 8-hydroxyadenine, 2,6-diamino-4-hydroxy-5-formamidopyrimidine and 8hydroxyguanine were identified as base products in DNA, and their yields were measured. These products are the typical hydroxyl radical-induced products of DNA bases, which are well known from the radiation chemistry of DNA in aqueous solution. This fact suggests that they were likely due to hydroxyl radicals produced in the neutrophil system.

PB92-117399 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Chemical Thermodynamics Thermodynamics of the Disproportionation of Adenosine 5'-diphosphate to Adenosine 5'-triphosphate and Adenosine 5'-monophosphate. 2. Experimental Data. Final rept.

Y. B. Tewari, R. N. Goldberg, and J. V. Advani. 1991,

See also PB92-116854. Pub. in Biophysical Chemistry 40, p163-176 1991.

Keywords: \*Thermodynamic equilibrium, \*Blood cells, \*Disproportionation, \*Magnesium ions, \*Adenosine phosphates, Liquid column chromatography, Calorimetry, Enthalpy, Entropy, ADP, Enzymes, Catalysts, Biochemistry, ATP, Temperature dependence, AMP, Measurement, pH, Hydrolysis, Specific heat, Activity coefficients, Bengints coefficients, Reprints.

High-pressure liquid-chromatography and microcalorimetry have been used to determine equilibrium constants and enthalpies of reaction for the disproportion reaction of adenosine 5'-diphosphate (ADP) to adeno-sine 5'-triphosphate (ATP) and adenosine 5'-mono-phosphate (AMP). Adenylate kinase was used to cataphosphate (AMP). Adenylate kinase was used to catalyze the reaction. The measurements were carried out over the temperature range 286 to 311 K, at ionic strengths varying from 0.06 to 0.33 mol/kg, over the PH range 6.04 to 8.87, and over the pMg range 2.22 to 7.16, where pMg = - log a(Mg (sup 2+)). The equilibrium model developed by Goldberg and Tawari was used for the analysis of the measurements. For the reference reaction: 2 ADP (3-)(a o) to AMP (2-)(ao) + ATP(4-)(ao), K=0.225 + or - 0.010, Delta G = 3.70 + or - 0.11 kJ/mol, Delta H = -1.5 + or - 1.5 kJ/mol, Delta 5 = -17 + or - 5 J/mol/K and Delta C(sub p) = -46 J/mol/K at 298.15K and 0.1 MPa. These results and the thermodynamic parameters for the auxiliary equilibria in solution have been used to model the thermodynamics of the disproportionation reaction over a modynamics of the disproportionation reaction over a wide range of temperature, pH, ionic strength, and magnesium ion molality. Under approximately physiological conditions (311.15 K. pH 6.94, (Mg(2+))=1.35 x 10(sup 3-) mol/kg, and I = 0.23 mol/kg) the apparent equilibrium constant for the overall disproportionation reaction is equal to 0.93 + or - 0.02. Thermodynamic data on the disproportionation reaction and literature of the content and interpretations. ature values for this apparent equilibrium constant in human red blood cells are used to calculate a molality of 1.94 x 10 (sup -4) mol/kg for free magnesium ion in human red blood cells. The results are also discussed in relation to thermochemical cycles and compared with data on the hydrolysis of the guanosine phosphates.

### Dentistry

101,314 PB91-187666

(Order as PB91-187617, PC A06/MF A01) National Inst. of Standards and Technology, Gaithersburg, MD.

Digital Image Analysis Assisted Microradiography Measurement of Mineral Content of Caries Lesions in Teeth.

C. Chow, S. Takagi, W. Tung, and T. H. Jordan. 1991, 12p

Prepared in cooperation with American Dental Association Health Foundation, Chicago, IL. Included in Jnl. of Research of the National Institute of Standards and Technology, v96 n2 p203-214 Mar/Apr

Keywords: \*Dental caries, \*Microradiography, \*Image analysis, Digital data, Lesions, Measurement, Thickness, Mineral content, Remineralization.

The study investigated the feasibility of using a digital image analysis system to process the information contained in microradiographs of tooth sections that included dental caries lesions. The results show that by using an aluminum step wedge to provide a range of thickness standards and a sound area of the sample as an internal reference, data on tooth mineral content as a function of the location can be obtained with an estimated error of less than 5% relative to the mineral content of sound area. The microradiographic technique allows the response of tooth samples to a remineralization treatment to be quantitatively measured and statistically analyzed.

101.315 PB91-194746 Not available NTIS National Inst. of Standards and Technology (IMSE), Gaithersburg, MD. Polymers Div. Effects of pH and Calcium on Hydrolysis of Na2SiF6 and Na2SnF6: A Quasi-Constant Composition Titration Study. Final rept.

N. Eidelman, and L. C. Chow. 1991, 7p Sponsored by American Dental Association Health Foundation, Chicago, IL. Pub. in Caries Research 25, p101-107 1991.

Keywords: \*Dental caries, \*Calcium ions, \*Reaction kinetics, \*Hydrolysis, \*Acid resistance, pH, Calcium phosphates, Titration, Surface chemistry, Inhibitors, Tin compounds, Fluoridation, Reprints, Sodium hexafluorostannate, Sodium hexafluorosilicate.

Hydrolysis reactions of sodium hexafluorosilicate (Na2SiF6) and sodium hexaflurostannate (Na2SnF6) were studied at various combinations of pH and calcium ion (Ca(2+)) concentrations using a quasi-constant composition titration method. Under high constant composition titration method. Under high con-centrations of hydrogen ion and Ca(2+), the promoting effect of Ca(2+) on the hydrolysis of Na2SiF6 was stronger than the inhibition effect of hydrogen ion. However, the inhibition effect of hydrogen ion on the hydrolysis of Na2SnF6 was stronger than the promot-ing effect of Ca(2+). Na2SiF6 and Na2SnF6 were found to have hydrolysis properties that may make them suitable for use with an acidic calcium phosphate solution in a topical fluoride treatment which forms dicalcium phosphate dihydrate as an intermediate.

### **MEDICINE & BIOLOGY**

# Dentistry

101,316 PB92-126689

(Order as PB92-126614, PC A06/MF A02) National Inst. of Standards and Technology, Gaithersburg, MD.

Mathematical Model for Dental Caries: A Coupled Dissolution-Diffusion Process.

T. M. Gregory, L. C. Chow, and C. M. Carey. 1991,

12p Included in Jnl. of Research of the National Institute of Standards and Technology, v96 n5 p593-604 Sep/Oct

Keywords: \*Dental caries, \*Teeth, Diffusion, Hydroxy compounds, Apatites, Computerized simulation, Demineralizing, Dissolution, Mathematical models, Thermodynamic equilibrium, Calcium ions, Phosphates, pH, Plaque formation, Membranes.

Demineralization of tooth mineral in the caries process was studied using a computer model that simulates a diffusion controlled dissolution process. The solution in the inner ('lesion') compartment was in equilibrium with the tooth mineral, but its composition changed in response to diffusion of ions between the two solutions through an infinitely thin barrier. A steady state condition is eventually reached under which the ratio of flux of Ca to that of P becomes 5/3. The results of the simulation show that for a given 'plaque' pH, the rate of demineralization at steady state was the highest for cation and the lowest for anion permselective membranes.

### Nutrition

PB91-147413 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Inorganic Analytical Research Div. Dietary Collection Procedures.

Final rept.

G. V. Iyengar. 1987, 7p

Pub. in Clinical Nutrition 6, n4 p147-153 Jul/Aug 87.

Keywords: \*Food analysis, \*Standards, Food consumption, Chemical analysis, Nutritive value, Diets, Nutrition.

There is no single method that may be regarded as entirely satisfactory for the purpose of estimating the human dietary intake of nutrients and toxic substances in foods, since each approach has some limitation or the other. Yet, many decisions of public health concern need to be made with analytical information available from ongoing biomedical trace element research studies. Therefore, every effort should be made to generate reliable analytical data from these investigations. More efforts are urgently needed to develop several kinds of dietary reference materials and to promote their use in standardizing analytical procedures in the food analysis laboratories if the results generated from field studies are to be used for the development of newer concepts for improving the currently used dietary intake models and to provide new guidelines

101.318 PB91-147421 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Inorganic Analytical Research Div.

Practical Constraints in Monitoring Micronutrient

Intake.

Final rept. G. V. lyengar. 1987, 5p

Pub. in Clinical Nutrition 6, n4 p154-158 Jul/Aug 87.

Keywords: \*Trace elements, \*Monitoring, Chemical analysis, Nutrition, Nutritive value, Diets, Food consumption, \*Biomonitoring.

Monitoring of human subjects for the daily intake of essential and toxic trace elements poses certain inherent difficulties. The reasons include, among others (1) there are only a few situations in which a direct asso-ciation between specific elements, target specimens, and dietary intake have been established, and (2) in many other situations, meaningful information can be derived only when simultaneous analyses of several different specimens from the same subject has been carried out. It is important to recognize that solutions to many of the biomonitoring type of problems require a

multidisciplinary approach to the problem as a whole, a sound understanding of the metabolic roles played by each element, as well as the gastrointestinal absorption properties as observed from different kinds of

### Pharmacology & Pharmacological Chemistry

101.319

PB91-195149 Not available NTIS National Inst. of Standards and Technology (IMSE), Gaithersburg, MD. Polymers Div.

Adsorption and Orientation of Tetracycline on Hydroxyapatite.

Final rept.

D. N. Misra. 1991, 6p

Sponsored by American Dental Association Health Foundation, Chicago, IL.

Pub. in Calcified Tissue International 48, p362-367

Keywords: \*Hydroxy compounds, \*Apatites, \*Tetracyclines, \*Separation processes, Adsorbents, Calcifica-tion, Bone, Teeth, Polymers, Orientation, Tissues, Eth-anols, Chloromethanes, Surface chemistry, Hydrogen bonds, Reprints.

Adsorption of tetracycline from separate solutions of ethanol, p-dioxane, and chloroform onto synthetic hy-droxyapatite (containing about 1.5 monolayer of physi-sorbed water) was studied in order to understand its interaction with bone and teeth. The adsorption isotherms of tetracycline are reversible and Langmuirian from ethanol and p-dioxane and are almost identical. The isotherm is irreversible from chloroform, and a constant amount of adsorbate is removed from the solutions above a certain concentration. An analysis of the reversible isotherms showed that at maximum coverage the ring or polycyclic structure of the molecule stands perpendicular to the surface with appropriate hydroxyl groups and ketooxygens hydrogen bonded to the surface. The process of adsorption does not affect the chemical integrity of tetracycline.

### Public Health & Industrial Medicine

101,320

PB91-204099 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Gas and Particulate Science Div.

Visibility of Chrysotile Asbestos in the Scanning Electron Microscope.

Final rept.

J. A. Small. 1985, 18p

Sponsored by Ontario Research Foundation, Mississauga.

Pub. in Proceedings of Workshop on Asbestos Fibre Measurements in Building Atmospheres, Toronto, Canada, March 1985, p69-86.

Keywords: \*Asbestos, \*Scanning electron microscopy, \*Visibility, Contrast, Chemical analysis, Fibers, Resolution, Reprints, \*Chrysotile.

Most manufacturers of conventional scanning electron microscopes (SEM)s claim resolution of the order of 3-10 nm for their instruments which is substantially less than the diameters of 20-30 nm reported for single-fibril chrysotile. With this level of resolution, it appears that these instruments should be able to image single fibrils of chrysotile asbestos under normal operating conditions in a real-time imaging mode appropriate to rapid sample searching. The limiting resolution per-formance of an SEM however can only be realized with an ideal high contrast sample such as a thin edge or a atrongly scattering particle viewed against a weakly scattering background. In anlayzing a material such as chrysotile asbestos with a low electron scattering coefficient, the visibility of chrysotile asbestos fibers is limited by the contrast of the sample rather than the ulti-mate resolution of the SEM used for the analysis.

# Radiobiology

101,321

PB91-190108 Not available NTIS National Inst. of Standards and Technology (CSTL),

Gaithersburg, MD. Biotechnology Div.
Mechanistic Studies of Ionizing Radiation and Oxidative Mutagenesis: Genetic Effects of a Single 8-Hydroxyguanine (7-Hydro-8-oxoguanine) Residue Inserted at a Unique Site in a Viral Genome. Final rept.

M. L. Wood, M. Dizdaroglu, E. Gajewski, and J. M. Essigmann. 1990, 9p Pub. in Biochemistry 29, n30 p7024-7032 1990.

Keywords: \*Ionizing radiation, \*Mutagenesis, \*Viral genes, DNA adducts, Escherichia coli, High pressure liquid chromatography, Mass fragmentography, Ultraviolet spectroscopy, T phages, Phosphorylation, Codon, Polyribonucleotide synthetase, Mutation, Reprints, \*8-hydroxyguanine.

T4 RNA ligase was used to construct a deoxypentanu-T4 RNA ligase was used to construct a deoxypentanucleotide containing a single 8-hydroxyguanine (7-hydro-8-oxoguanine; G(sup 8-OH)) residue, which is one of the putatively mutagenic DNA adducts produced by oxidants and ionizing radiation. The pentamer d(GCTAG(sup 8-OH)p was prepared by the ligation of a chemically synthesized acceptor molecule, d(GCTA), to an adducted donor, 8-hydroxy-2'-deoxyguanosine 5',3'-bisphosphate. The acceptor was efficiently converted to the reaction product (>95%), and the final product yield was 50%. Following 3'-dephosphorylation, the pentamer was characterized by UV phorylation, the pentamer was characterized by UV pholylation, the peritainer was characterized by Ov spectroscopy, by high-pressure liquid chromatogra-phy, and by gas chromatography-mass spectrometry of the nucleosides released by enzymatic hydrolysis. Both d(GCTAG(sup 8-OH) and an unmodified control were 5'-phosphorylated by using (gamma-32P) ATP and incorporated covalently by DNA ligase into a fivebase gap at a unique Nhel restriction site in the other duplex genome of an M13mp19 derivative. The ligation product contained G(sup 8-OH) at the 3' residue of an in-frame amber codon (5'-TAG-3') (genome position 6276) of the phage lacZa gene. The adduct was part of a nonsense codon in a unique restriction site in order to facilitate the identification and selection of mutants generated by the replication of the modified genome in Escherichia coli.

101,322

Not available NTIS PB91-195057 National Inst. of Standards and Technology (NML), Gaithersburg, MD. Ionizing Radiation Div. Absorbed Dose to Water: Comparison of Several

Methods Using a Liquid Ionization Chamber. Final rept.

O. Mattsson, H. Svensson, G. Wickman, S. R. Domen, J. S. Pruitt, and R. Loevinger. 1990, 6p Sponsored by Sahlgren Hospital, Gothenburg (Sweden), and Umea Univ. (Sweden). Pub. in Acta Oncologica 29, n2 p235-240 1990.

Keywords: \*Radiation doses, Liquid ionization chambers, Iron sulfates, Gamma rays, Calorimeters, Dosimetry, Comparison, Water, Reprints.

A liquid ionization chamber has been used as a transfer instrument for the quantity absorbed dose to water in a cobalt-60 gamma ray beam. The characteristics of the liquid ionization chamber are described. The transferred dosimetric information has been compared with absorbed dose determinations using air ionization chamber dosimetry, water calorimetry and ferrous sulphate dosimetry. The agreement between the different measured absorbed dose values is very good, i.e., within 0.2%. This is an indication that the consistency in the methods to determine absorbed dose to water is good. The impact of the new standard for air-kerma, introduced in 1986 by the BIPM, on the air ionization chamber is investigated. It is shown that any differences in the dosimetry when using the old or the new set of data cancel out for the cobalt-60 beam. The investigation also shows that the value of (epsilon sub for the ferrous sulphate dosimeter recommended in ICRU 35 for electrons can be used also in the cobalt-60 beams.

101.323

PB91-203265 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Ionizing Radiation Div.

Interlaboratory Comparison of Actinides in Human Tissue (239)Pu  $\,+\,$  (240)Pu.

Final rept.
K. G. W. Inn, W. S. Liggett, H. L. Volchok, M. S. Feiner, J. F. McInroy, D. S. Popplewell, D. R. Percival, R. A. Wessman, V. T. Bowen, H. D. Livington, R. L. Kathren, and H. Kawamura. 1990,

Pub. in Jnl. of Radioanalytical and Nuclear Chemistry 138, n2 p219-229 1990.

Keywords: \*Actinides, \*Tissues(Biology), \*Plutonium 239, \*Plutonium 240, \*Interlaboratory comparisons, Humans, Reprints, Standard Reference Materials.

An international laboratory intercomparison of actinides in human tissues was organized by the United States Transuranic Registry and the National Bureau of Standards. Five laboratories from the United States, United Kingdom, and Japan participated in the intercomparison. The laboratories were requested to analyze Standard Reference Materials 4351 (Human Lung) and 4352 (Human Liver) for (239)Pu + (240)Pu concentration. In general, approximately equivalent measurement capabilities were found among the participants. The results of the intercomparison were statistically comparable to those used for the original cer-tification of the SRMs, and were combined for a reevaluation of the certified values. The sum of the data sets resulted in notable improvements in the certification for the plutonium content in these SRMs.

#### 101,324

PB91-236497 Not available NTIS

National Inst. of Standards and Technology (PL), Gaithersburg, MD. Ionizing Radiation Div.

Use of Storage Phosphor Imaging Plates in Portal Imaging and High-Energy Radlography: The Intensifying Effect of Metallic Screens on the Sensitivity. ty. Final rept.

Roehrig, C. E. Dick, and R. C. Placious. 1991, 7p Pub. in Medical Physics 18, n3 p432-438 May/Jun 91.

Keywords: \*Biomedical radiography, \*Dosimetry, \*Phosphors, \*Nuclear medicine, Sensitivity, Metals, Images, Radiation transport, Photon beams, Cobalt 60, Spectrum analysis, Radiation doses, Monte Carlo method, Reprints.

The sensitivity of storage phosphor imaging plates (SPIP) at megavolt photon energies (Cobalt 60, 6-, 10-, and 18-MV radiotherapy beams) is studied both experimentally and by Monte Carlo radiation transport calculations. In addition, the same techniques are used to investigate the intensifying effect of metal screens on the sensitivity of the SPIP. The results provide evi-dence that the sensitivity of the SPIPs is proportional to the absorbed energy in the phosphor layer per cGy. The spectral sensitivity is calculated for photon energies between 10 keV and 20 MeV for various SPIPscreen combinations.

### 101,325

PB91-236877 Not available NTIS National Inst. of Standards and Technology (PL), Gaithersburg, MD. Ionizing Radiation Div. Biomarkers of OH Radical Damage In vivo.

Final rent

L. R. Karam, D. S. Bergtold, and M. G. Simic. 1991, Sponsored by Defense Nuclear Agency, Washington,

Pub. in Free Rad. Res. Comms. 12-13, p11-16 1991.

Keywords: \*Chemical radiation effects, \*Free radicals, \*Hydroxyl radicals, \*In vivo, \*Biological effects, Mechanism, Synthesis(Chemistry), Tyrosine, Thymine, Glycols, Urine, Biological markers, Reprints.

Mechanisms of formation of o-tyrosine (o-Tyr) and thymine glycol (TG), the two possible markers of OH radical generation in biosystems and in vivo are described. The o-Tyr measurements require invasive approaches, while TG detection may be accomplished by noninvasive analysis in the urine.

# 101,326

Not available NTIS PB91-237008 National Inst. of Standards and Technology (PL), Gaithersburg, MD. Ionizing Radiation Div.

Sensitometry of the Response of a New Radiochromic Film Dosimeter to Gamma Radiation and Electron Beams. Final rept.

W. L. McLaughlin, C. Yun-Dong, C. G. Soares, A. Miller, G. Van Dyk, and D. F. Lewis. 1991, 12p Pub. in Nuclear Instruments and Methods in Physics Research A302, p165-176 1991.

Keywords: \*Dosemeters, \*Film dosimetry, \*Gamma rays, \*Electron beams, Biomedical radiography, Industrial radiography, Images, Irradiation, Nondestructive tests, Sensitivity, Spectrum analysis, Temperature dependence, Reprints.

new radiation-sensitive imaging material, called GafChromic (TM) Dosimetry Media, offers advances in high-dose radiation dosimetry and high-resolution radiography for gamma radiation and electrons. The potential uses in radiation processing, radiation sterilization of medical devices, population control of insects by irradiation, food irradiation, blood irradiation for organ-transplant immuno-suppression, clinical radiography, and industrial radiography have led to the present sensitometric study over the breadth of the wide dynamic range of the new routine detector and imaging material, namely, absorbed doses from 10 Gy to 5 x 10 to the 4th power Gy. The thin-coated film is colorless before irradiation, and registers a deep-blue image upon irradiation, with two absorption bands at about 650 nm (major band) and 600 nm (minor band). The response to electrons, in terms of increase in absorbance per unit absorbed dose, is the same as that to gamma radiation within the estimated uncertainty of the measurements (+ or - 5%, 95% confidence level). The spatial resolving power is > 1200 lines/mm. After the first 24 hours, the image is stable over many months (within + or - 5% in absorbance), however, the system should be irradiated and analyzed at approximately the temperatures used during calibration, because of temperature dependence during irradiation and readout, and temperatures greater than 55 C should be avoided.

101,327 PB91-237388 Not available NTIS National Inst. of Standards and Technology (PL), Gaithersburg, MD. Ionizing Radiation Div. Calibration of Ophthalmic Applicators at NIST: A Revised Approach.

Final rept. C. G. Soares. 1991, 7p Pub. in Medical Physics 18, n4 p787-793 Jul/Aug 91.

Keywords: \*Radiation doses, \*Calibrating, \*Film dosimetry, \*Opthalmology, \*Beta dosimetry, Electric currents, Extrapolation chambers, Irradiation, Spectrum analysis, Measurement, US NBS, Reprints, \*Ophthamic applicators.

A revised approach to the problem of measuring a surface-absorbed dose from beta-particle-emitting oph-thalmic applicators is presented. The technique chosen employs an extrapolation chamber equipped with a 4-mm-diam collecting electrode to make current measurements at air gaps from 0.08 to 0.20 mm at 0.02-mm intervals. These data yield a linear relationship between current and air gap, the slope of which is used to determine average surface-absorbed-dose rate over the central area of the source. For additional information about the distribution of the activity over the source surface, autoradiographs using calibrated radiochromic dye films are analyzed to map the doserate profile across the surface of the applicator. Experiments varying several parameters of the extrapolation chamber measurement, including collecting electrode area, voltage gradient, range of air gaps used, and entrance foil material, are described. Also treated are calibrations of, and a description of the use of, radiochromic dye films for source profiling. Experiments for determining correction factors for the extrapolation chamber measurements are described, and an assessment of the uncertainties associated with these measurements is given.

### **Toxicology**

101,328 Not available NTIS PB91-162032 National Inst. of Standards and Technology (IMSE), Gaithersburg, MD. Polymers Div.

Newest Approaches to Quantitative Assessment of Bioactive Organotins.

Final rept.

I. C. Felkner, B. Worthy, G. J. Olson, and F. E.

Brinckman, 1989, 14p Pub, in Chemical Speciation and Bioavailability 1, n3 p79-92 Oct 89.

Keywords: \*Organotin compounds, \*Bacillus subtilis, \*Toxicity, Bioassay, Lasers, Genetic engineering, Reprints, \*Toxic substances.

New approaches for assessing the toxicity of organo-tin chemical species have been developed. These approaches are based upon the selective responses of sensitive biodetectors whose chemical and molecular interactions with a wide variety of toxicants have been previously determined and reported. Bioassays capable of quantitating and chemically speciating toxicants for impacts on diverse bacterial sensors are discussed herein. The principal new development is a laser/bacterial bioassay which is capable of differentiating between various toxic chemicals and specifically distinguishing between the different organotin species based on their mechanism of toxic action. The system uses a battery of isogenic Bacillus subtilis strains genetically engineered to respond differentially to specific toxicants. The response is monitored by differential light scattering of a laser which is integrated with a computerized system that collects and analyzes the data. The system routinely generates fully analyzed data within 66 min for most samples. It is capable of making 1,200 measurements on each sample within 2 to 4 seconds, and shows promise as a rapid and inexpensive system to monitor organotins and various other toxicants on site.

101.329

PB91-187070 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Chemical Kinetics Div. Base Modifications in Plasmid DNA Caused by Po-

tassium Permanganate. Final rept.

S. A. Akman, J. Doroshow, and M. Dizdaroglu. 1990,

Pub. in Archives of Biochemistry and Biophysics 282, n1 p202-205 Oct 90.

Keywords: \*Plasmids, \*Deoxyribonucleic acids, \*Potassium permanganate, \*DNA damage, \*Toxicity, Mass fragmentography, Mutagenicity tests, Cell survival, lons, Reprints.

KMnO4 is a powerful oxidizing agent which has been used to modify DNA bases. In previous studies, mild KMnO4 treatment has been shown to preferentially modify the treatment has been shown to preferential modify Thy, Cyt and Gua are modified only under harsher conditions to as yet unidentified products. In the present study, denatured plasmid pCMV beta gal DNA was exposed to 0.015-1.5 mM KMnO4, pH 8.6, at 4 C for 5 min, after which the DNA was hydrolyzed in formic acid, trimethylsilylated, and analyzed for modified base content by gas chromatography-mass spec-trometry/selected ion monitoring. The study data sug-gest that previous studies which have used treatment with KMnO4 to study the mutagenicity of Thy glycol specifically or as a Thy-specific probe in DNA structure should be interpreted with caution.

101.330

PB91-187104 Not available NTIS National Inst. of Standards and Technology (CSTL), Gaithersburg, MD. Biotechnology Div.

Copper-Ion-Dependent Damage to the Bases in DNA in the Presence of Hydrogen Peroxide. Final rept.

O. I. Aruoma, B. Halliwell, E. Gajewski, and M. Dizdaroglu. 1991, 4p Pub. in Biochemistry Jnl. 273, p601-604 1991.

Keywords: \*DNA damage, \*Hydrogen peroxide, \*Toxicity, \*Copper, \*Iron, Ions, Hydroxyl radicals, Catalase, Superoxide dismutase, Ascorbic acid, Reprints, Hypoxanthine-xanthine oxidase system.

Mixtures of Cu(sup 2+) and H2O2 at pH 7.4 caused damage to the bases in DNA greater than that caused by mixtures of Fe(Sup 3+) and H2O2. Addition of ascorbic acid to the Cu(Sup 2+)/H2O2 system caused a very large increase in base damage, much greater than that produced by the Fe(sup 3+)/H2O2/ ascorbic acid system. The products of base damage in the presence of Cu(sup 2+) were typical products that have been shown to result from attack of hydroxyl radi-

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cals upon the DNA bases. Cytosine glycol, thymine glycol, 8-hydroxyadenine and especially 8-hydroxy-guanine were the major products in both the Cu(sup 2+)/H2O2 and the Cu(sup 2+)/H2O2/ascorbic acid systems. Base damage in DNA by these systems was inhibited by the chelating agents EDTA and nitrilotria-cetic acid and by catalase, but not by superoxide dis-mutase, nor by the hydroxyl-radical scavenger mannitol. It is proposed that Cu(sup 2+) ions bound to the DNA react with H2O2 and ascorbic acid to generate hydroxyl radicals, which then immediately attack the DNA bases in a site-specific manner. A hypoxanthine/ xanthine oxidase system also caused damage to the DNA bases in the presence of Cu(sup 2+) ions. This was inhibited by superoxide dismutase and catalase. The high activity of Cu(sup 2+) ions, when compared with Fe(sup 3+) ions, in causing hydroxyl-radical-dependent damage to DNA and to other biomolecules, means that the availability of Cu(sup 2+) ions in vivo must be carefully controlled.

101,331 PB91-187112 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Chemical Kinetics Div. Damage to the Bases in DNA Induced by Hydrogen Peroxide and Ferric Ion Chelates. Final rept.

O. I. Aruoma, B. Halliwell, E. Gajewski, and M.

Dizdaroglu. 1989, 4p Pub. in Jnl. of Biological Chemistry 264, n34 p20509-20512, 5 Dec 89.

Keywords: \*DNA damage, \*Hydrogen peroxide, \*Iron, \*Chelating agents, Toxicity, Hydroxyl radicals, Enzyme inhibitors, Superoxide dismutase, Carcinogens, inhibitors, Superoxide dismutase, Carolings..., Kidney, Reprints, Hypoxanthine-xanthine oxidase

Incubation of a number of ferric ion chelates with H2O2 at pH 7.4 generated a reactive species able to produce chemical modifications of the bases in DNA that are very similar to those produced in DNA by the hypoxanthine/xanthine oxidase system. Products were identified and quantitated by the use of gas chromatography-mass spectrometry with selected-ion monitoring. Compared with other complexes used, ferric ion-nitrilotriacetic acid produced by far the largest amount of the base products. Typical hydroxyl radical scavengers and superoxide dismutase provided significant decreases in the yields of the products. On this basis, it is proposed that ferric ion complexes react with H2O2 to produce hydroxyl radical; this was also shown using the deoxyribose assay.

101,332 PB91-187468 Not available NTIS National Inst. of Standards and Technology (CSTL), Gaithersburg, MD. Biotechnology Div.

Chemical Determination of Free Radical-Induced

Damage to DNA. Final rept.

Fillian Tept. M. Dizdaroglu. 1991, 18p Sponsored by Department of Energy, Washington, DC. Pub. in Free Radical Biology and Medicine 10, p225-

Keywords: \*Free radicals, \*DNA damage, \*Toxicity, Mass fragmentography, Hydroxyl radicals, Cross-linking reagents, Histones, Chromatin, Mammals, Re-

Free radical-induced damage to DNA in vivo can result in deleterious biological consequences such as the initiation and promotion of cancer. Chemical characterization and quantitation of such DNA damage is essential for an understanding of its biological consequences and cellular repair. Methodologies incorporating the technique of gas chromatography/mass spectaremetry. (GC/MS) have been developed in secret trometry (GC/MS) have been developed in recent years for measurement of free radical-induced DNA damage. The use of GC/MS with selected ion monitoring (SIM) facilitates unequivocal identification and quantitation of a large number of products of all four DNA bases produced in DNA by reactions with hydroxyl radical, hydrated electron, and H atom. Hydroxyl radical-induced DNA-protein cross-links in mammalian chromatin, and products of the sugar moiety in DNA are also unequivocally identified and quantified. The sensitivity and selectivity of the GC/MS-SIM technique enables the measurement of DNA base products even in isolated mammalian chromatin without the necessity of first isolating DNA, and despite the presence of histones. Recent results demonstrate the usefulness of the GC/MS technique for chemical determination of free radical-induced DNA damage in DNA as well as in

mammalian chromatin under a vast variety of conditions of free radical production.

101.333

PB91-187492 Not available NTIS National Inst. of Standards and Technology (CSTL), Gaithersburg, MD. Biotechnology Div. Modification of Bases in DNA by Copper Ion-1,10-

Phenanthroline Complexes.

M. Dizdaroglu, O. I. Aruoma, and B. Halliwell. 1990,

Pub. in Biochemistry 29, n36 p8447-8451 1990.

Keywords: \*DNA damage, \*Toxicity, Superoxide, Pyrimidines, Purines, Hydroxyl radicals, Catalase, Dimethyl sulfoxide, Reprints, Copper ion-phenanthroline com-

Damage to the bases in DNA by the cupric ion-1,10phenanthroline complex was investigated. Ten base products in DNA were identified and quantitated by the use of gas chromatography/mass spectrometry with selected-ion monitoring. DNA damage by the cupric ion-1,10-phenanthroline complex required the presence of a reducing agent such as ascorbic acid or mercaptoethanol. Products identified were typical hydroxyl radical induced products from the pyrimidines and purines in DNA, well-known from previous studies using various hydroxyl radical producing systems such as ionizing radiation, hypo-xanthine/xanthine oxidase, or hydrogen peroxide in the presence of transition metal ions. Product formation was not significantly inhibited by typical scavengers of hydroxyl radical such as mannitol and sodium formate, but there was partial inhibition by dimethyl sulfoxide. Catalase substantially decreased formation of base products, and added hydro-gen peroxide stimulated it, indicating the hydrogen peroxide dependency of DNA base damage. Superoxide dismutase afforded only a partial reduction in product yields in systems containing ascorbic acid. On the basis of the types of base products formed, the hydrogen peroxide dependency of product formation, and a previous report suggesting that DNA damage is due to a diffusible species the study suggests that DNA base damage is caused by hydroxyl radical.

101.334

PB91-187518 Not available NTIS National Inst. of Standards and Technology (CSTL), Gaithersburg, MD. Biotechnology Div. Structure and Mechanism of Hydroxyl Radical-Induced Formation of a DNA-Protein Cross-Link Involving Thymine and Lysine in Nucleohistone. Final rept.

M. Dizdaroglu, and E. Gajewski. 1989, 5p Pub. in Cancer Research 49, p3463-3467, 1 Jul 89.

Keywords: \*DNA damage, \*DNA-binding proteins, \*Thymine, \*Lysine, \*Hydroxyl radicals, \*Toxicity, Mass fragmentography, Cross-linking reagents, Amino fragmentography, Cross-linking acids, Reprints, \*Nucleohistones.

Hydroxyl radical-induced formation of a DNA-protein cross-link involving thymine and lysine in calf thymus nucleohistone in vitro is reported. Basic amino acids such as lysine constitute a very high proportion of the amino acids of histones, and help histones to bind to DNA in chromatin. For this reason, basic amino acids are likely to participate in DNA-protein cross-linking. For identification of the thymine-lysine cross-link in nu-cleohistone, hydroxyl radical-induced cross-linking of thymine to lysine was investigated first using a model system, i.e., an aqueous mixture of thymine and lysine. Hydroxyl radicals were generated by exposure of the mixture to ionizing radiation after N2O saturation. The technique of gas chromatography-mass spectrometry was used to analyze the samples for possible cross-links. One thymine-lysine cross-link was found and its structure was elucidated. Using gas chromatography-mass spectrometry with selected-ion monitoring, this thymine-lysine cross-link was identified in acidic hydro-lysates of calf thymus nucleohistone gamma-irradiated in N2O-saturated aqueous solution.

101,335

Not available NTIS National Inst. of Standards and Technology (CSTL), Gaithersburg, MD. Biotechnology Div. Chemical Nature of In vivo DNA Base Damage in Hydrogen Peroxide-Treated Mammalian Cells. Final rept.

M. Dizdaroglu, Z. Nackerdien, B. C. Chao, E. Gajewski, and G. Rao. 1991, 3p Sponsored by Department of Energy, Washington, DC., and National Science Foundation, Washington, DC:

Pub. in Archives of Biochemistry and Biophysics 285, n2 p388-390 Mar 91.

Keywords: \*DNA damage, \*Hydrogen peroxide, \*Toxicity, Mammals, Cells(Biology), In vivo analysis, Mass fragmentography, Hydroxyl radicals, Chromatin, Re-

Hydrogen peroxide is generated in mammalian cells by normal metabolism or by treatment with external agents. Treatment of mammalian cells with this oxidizing agent results in DNA damage. Little is known about the chemical nature of hydrogen peroxide-mediated DNA damage in mammalian cells. The study reports on the chemical characterization of in vivo base damage to nuclear DNA in mammalian cells caused by exposure to H2O2. Chromatin was isolated from cells and analyzed by gas chromatography/mass spectrometry with selected-ion monitoring. Ten DNA base products were identified and quantitated. Modified bases identified were typical hydroxyl radical-induced products of DNA bases. Results indicate involvement of hydroxyl radicals in the mechanism of nuclear DNA damage in mammalian cells caused by H2O2.

PB91-189217 PB91-189217 Not available NTIS National Inst. of Standards and Technology (CSTL),

Gaithersburg, MD. Biotechnology Div. Damage to the DNA Bases in Mammalian Chromatin by Hydrogen Peroxide in the Presence of Ferric and Cupric Ions. Final rept.

M. Dizdaroglu, G. Rao, B. Halliwell, and E. Gajewski.

Sponsored by Department of Energy, Washington, DC Pub. in Archives of Biochemistry and Biophysics 285, n2 p317-324 Mar 91.

Keywords: \*DNA damage, \*Chromatin, \*Hydrogen peroxide, \*Iron, \*Copper, \*Toxicity, Cations, Mammals, Superoxide dismutase, Hydroxyl radicals, Re-

Modification of DNA bases in mammalian chromatin upon treatment with hydrogen peroxide in the pres ence of ferric and cupric ions was studied. Ten DNA base products in mammalian chromatin were identified and quantitated by the use of gas chromatographymass spectrometry with selected-ion monitoring after hydrolysis of chromatin and trimethylsilylation of hydrolysates. Hydrogen peroxide in the presence of cupric ions caused more DNA damage than in the presence of ferric ions. Chelation of cupric ions caused a marked inhibition in product formation. By contrast, DNA was damaged more extensively in the presence of chelated ferric ions than in the presence of unchelated ferric ions. The presence of ascorbic acid generally increased the yields of the products, indicating increased production of hydroxyl radical by reduction of metal ions by ascorbic acid.

PB91-189357 Not available NTIS National Inst. of Standards and Technology (CSTL), Gaithersburg, MD. Biotechnology Div. Bleomycin-Dependent Damage to the Bases in

DNA Is a Minor Side Reaction. Final rept.

E. Gajewski, O. I. Aruoma, M. Dizdaroglu, and B. Halliwell, 1991, 5p Pub. in Biochemistry 30, n9 p2444-2448 1991.

Keywords: \*Bleomycin, \*Toxicity, \*DNA damage, Antineoplastic agents, Gas fragmentography, Catalase, Hydroxyl radicals, Iron, Hydrogen peroxide, Superoxide dismutase, Thiobarbituric acid, Reprints.

The antitumor antibiotic bleomycin degrades DNA in the presence of ferric ions and H2O2 or in the presence of ferric ions, oxygen, and ascorbic acid. When DNA degradation is measured as formation of base propenals by the thiobarbituric acid assay, it is not inhibited by superoxide dismutase and scavengers of the hydroxyl radical or by catalase (except that cata-lase inhibits in the bleomycin/ferric ion/H2O2 system by removing H2O2). Using the technique of gas chro-

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matography/mass spectrometry with selected-ion monitoring, the study shows that DNA degradation is accompanied by formation of small amounts of modified DNA bases. The products formed are identical with those generated when hydroxyl radicals react with DNA bases. Base modification is significantly inhibited by catalase and partially inhibited by scavengers of the hydroxyl radical and by superoxide dismutase. The study suggests that the bleomycin-oxo-iron ion complex that cleaves the DNA to form base propenals can decompose in a minor side reaction to generate hydroxyl radical, which accounts for the base modification in DNA. However, hydroxyl radical makes no detectable contribution to the base propenal formation.

101,338 PB91-189373 Not available NTIS National Inst. of Standards and Technology (CSTL),

Gaithersburg, MD. Biotechnology Div.

Modification of DNA Bases in Mammalian Chromatin by Radiation-Generated Free Radicals.

E. Gajewski, G. Rau, Z. Nackerdien, and M. Dizdaroglu. 1990, 7p Pub. in Biochemistry 29, n34 p7876-7882 1990.

Keywords: \*DNA damage, \*Chromatin, \*Free radicals, \*Toxicity, \*Ionizing radiation, Mammals, Hydrolysis, Superoxide, Mass fragmentography, Reprints.

Modification of DNA bases in mammalian chromatin in aqueous suspension by ionizing radiation generated free radicals was investigated. Argon, air, N2O, and N2O/O2 were used for saturation of the aqueous system in order to provide different radical environments. Radiation doses ranging from 20 to 200 Gy (J/kg) were used. Thirteen products resulting from radical interactions with pyrimidines and purines in chromatin were identified and quantitated by using the technique of gas chromatography/mass spectrometry with selected-ion monitoring after acidic hydrolysis and tri-methylsilylation of chromatin. The methodology used permitted analysis of the modified bases directly in chromatin without the necessity of isolation of DNA from chromatin first. The results indicate that the radical environment provided by the presence of different gases in the system had a substantial effect on the types of products and their quantities. Some products were produced only in the presence of oxygen, where-as other products were detected only in the absence of oxygen. Products produced under all four gaseous conditions were also observed. Generally, the presence of oxygen in the system increased the yields of the products with the exception of formamidopyrimidines. Superoxide radical formed in the presence of air, and to a lesser extent in the presence of N2O/O2, had no effect on product formation.

**MILITARY SCIENCES** 

Logistics, Military Facilities, & Supplies

101.339 PB91-158832 Not available NTIS National Inst. of Standards and Technology (NCSL), Gaithersburg, MD. Information Systems Engineering

Data Management Standards in Computer-Aided Acquisition and Logistic Support (CALS).

Final rept. D. K. Jefferson. 1990, 30p

Pub. in Proceedings of Technology for Space Station Evolution Workshop, Dallas, TX., January 16-19, 1990,

Keywords: \*Logistics support, \*Computer applications, \*Data management, \*Standards, Federal information processing standards, Data bases, Query languages, Quality control, Reprints, IRDS(Information Resource Dictionary System), RDA(Remote Database Access), SQL.

The Computer-aided Acquisition and Logistic Support (CALS) initiative intends to replace the present flow of paper between islands of automation with, initially, digital data interchange, and, ultimately, an integrated shared database. These objectives can be attained in an open systems (non-proprietary) environment only through the use of national and international standards for data interchange and database. The presentation describes the current status and future expectations for the key database standards: the SQL family for database definition and manipulation; the IRDS family for metadata management; and the RDA family for data-base distribution. Together these standards will pro-vide a robust, flexible foundation for data management solutions to important national problems of efficiency and quality control.

101,340

PB91-167247 PC A05/MF A01 National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Center for Building Technology. Field Study of the Performance of EPDM Roofing at Air Force Facilities.

W. J. Rossiter, J. F. Seiler, W. P. Spencer, and P. E. Stutzman. Jan 91, 78p NISTIR-4504
Sponsored by Air Force Engineering and Services Center, Tyndall AFB, FL.

Keywords: \*Military facilities, \*Roofs, \*Inspection, Membranes, Performance, Mechanical tests, Field tests, Surveys, Defects, Adhesion, Seams(Joints).

A study was conducted at the request of the Air Force Engineering and Services Center to obtain and analyze information on the in-service performance of low-sloped EPDM roofing systems at Air Force installa-tions. Because of the benefits to be gained in having available alternative materials for fabricating membranes for low-sloped roofing systems, the Air Force has proposed developing a guide specification for EPDM roofing. Technical data are needed to support the development of the guide specification. The information obtained in the study contributes to the data base. Fifteen USAF installations in 11 states were visited, and 61 EPDM roofs were inspected. This represented about 50 percent of the number of Air Force installations and buildings with EPDM roofing. The age of the roof systems ranged from 3 to 156 months, although 40 percent were only 30 months old or less. The inspections were performed by walking over the roofs during which notes were recorded and photos were taken. During the field visits, discussions were held with base engineering personnel to determine their views of the performance of EPDM roofing under their responsibility. Considering the relatively young age of the roofs inspected, their overall performance was found to be satisfactory. About half were visually seen to be in fine condition, while another third dis-played only minor defects which were limited in scope and were considered to be readily reparable with routine maintenance. On a less positive note, in the latter case, the observed defects had gone without repair. This illustrated a key concern expressed by field personnel that they lacked ability to perform routine maintenance.

101,341

PB91-167296 PC A04/MF A01 National Inst. of Standards and Technology (NCSL), Raithersburg, MD.
Raster Graphics Conformance Testing.
F. E. Spielman. Feb 91, 54p NISTIR-4524

Keywords: \*Computer graphics, \*Sweep generators, \*Laboratories, \*Tests, Conformity, Standards, Evaluation, Programs, Management, \*Computer-aided Acquisition and Logistic Support, Department of Defense.

The report evaluates the alternatives for identifying and selecting a conformance testing laboratory for raster graphics in support of the Department of De-fense (DoD) Computer-aided Acquisition and Logistic

Support (CALS) Program. It discusses and analyzes four different approaches to selecting a conformance testing laboratory. After discussing the approaches, it recommends an alternative for DoD to pursue in selecting a laboratory for conducting conformance test-ing of raster graphics implementations. The annexes the report describe the requirements, procedures, forms, and criteria necessary for establishing and man-aging a raster graphics conformance testing program.

PB91-178889 PC A12/MF A02 National Inst. of Standards and Technology (NCSL), Gaithersburg, MD.

Collection of Technical Studies Completed for the Computer-Alded Acquisition and Logistic Support (CALS) Program. Fiscal Year 1988. Volume 1 of 3. Text, Security and Data Management.

Rept. for Oct 87-Sep 88. R. S. Morgan. Apr 90, 253p NISTIR-4315 See also PB91-178897 and PB91-178905. Sponsored by Assistant Secretary of Defense (Production and Logistics), Washington, DC. Computer-Aided Acquisition and Logistic Support Program.

Keywords: \*Data management, \*Text processing, \*Computer security, Publishing, Federal information processing standards, Computer graphics, Tests, \*CALS(Computer-aided Acquisition and Logistic Support), National Institute of Standards and Technology, PDÉS(Product Data Exchange Specification).

Computer-aided Acquisition and Logistic Support (CALS) Program is a Department of Defense (DoD) and Industry strategy to transition from paper-intensive acquisition and logistic processes to a highly automated and integrated mode of operation for the weapon systems of the 1990s. The three volumes of the report document and accomplishments of the National Institute of Standards and Technology (NIST) to advance the development of technology and standards in sup-port of CALS. In Volume 1, work on text and graphics standards in the CALS publishing environment is described, including technology assessments, applica-tion guidance, conformance test plans and a draft Fed-eral Information Processing Standard (FIPS) for ODA/ ODIF. Additionally, a technology assessment and proposed conformance testing strategy for page description management tools is presented with a discussion of computer security issues. The use of the Information Resource Dictionary System, (IRDS, ANSI Standard X3. 138-1988) is proposed as an integration and configuration management mechanism for the Product Data Exchange Specification (PDES).

PB91-178897 PC A21/MF A03 National Inst. of Standards and Technology (NCSL),

Gaithersburg, MD.
Collection of Technical Studies Completed for the Computer-Aided Acquisition and Logistic Support (CALS) Program, Fiscal Year 1988. Volume 2 of 3. Graphics, CGM MIL-SPEC.

Rept. for Oct 87-Sep 88.

R. S. Morgan. Mar 91, 482p NISTIR-4316 See also PB91-178889 and PB91-178905. Sponsored by Assistant Secretary of Defense (Production and Logistics), Washington, DC. Computer-Aided Acquisition and Logistic Support Program.

Keywords: \*Computer graphics, \*Standards, Tests, Inrecymores: Computer graphics, "Standards, Tests, Information systems, Data processing, Text processing, Protocols, "CALS(Computer-aided Acquisition and Logistic Support), National Institute of Standards and Technology, CGM(Computer Graphics Metafile), Department of Defense.

Computer-aided Acquisition and Logistic Support (CALS) Program is a Department of Defense (DoD) Industry strategy to transition from paper-intensive ac-quisition and logistic processes to a highly automated and integrated mode of operation for the weapon systems of the 1990s. The three volumes of the report document the accomplishments of the National Institute of Standards and Technology (NIST) to advance the development of technology and standards in sup-port of CALS. In Volume 2, progress in the Computer Graphics Metafile (CGM) standard is described, including work in the graphics standards committees and the expansion and updating of the CALS CGM application profile. A draft Military Specifications for CGM is included. A plan for Extended CGM is presented, including documentation of relevant standards committee

101,344 PB91-178905 PC A08/MF A01 National Inst. of Standards and Technology (NCSL), Gaithersburg, MD.

Collection of Technical Studies Completed for the Computer-Aided Acquisition and Logistic Support (CALS) Program, Fiscal Year 1988. Volume 3 of 3. CGM Registration.

Rept. for Oct 87-Sep 88.

R. S. Morgan. Apr 90, 173p NISTIR-4317
See also PB91-178897 and PB91-178889. Sponsored by Assistant Secretary of Defense (Production and Logistics), Washington, DC. Computer-Aided Acquisition and Logistic Support Program.

### **MILITARY SCIENCES**

# Logistics, Military Facilities, & Supplies

Keywords: Registration, Programming languages, Standardization, \*CALS(Computer-aided Acquisition and Logistic Support), \*CGM(Computer Graphics Metafile), National Institute of Standards and Technology.

Computer-aided Acquisition and Logistic Support (CALS) Program is a Department of Defense (DOD) and Industry strategy to transition from paper-intensive acquisition and logistic processes to a highly automated and integrated mode of operation for the weapon systems of the 1990s. The three volumes of the report document the accomplishments of the National Institute of Standards and Technology (NIST) to advance the development of technology and standards in support of CALS. Volume 3 documents work accom-plished to meet CALS needs for Computer Graphics Metafile (CGM) functionality through the registration of graphical elements within the standardization process.

101,345 PB91-184812 PC A03/MF A01 National Inst. of Standards and Technology (NCSL),

Gaithersburg, MD.
Standard Generalized Markup Language Encoding of the Office Document Architecture Document

Application Profile.
R. B. Wilson. Apr 91, 34p NISTIR-4547

Keywords: \*Information processing, \*Documents, Standards, Text processing, Logistics support, Computer applications, \*Computer-aided Acquisition and Logistic Support, \*SGML(Standard Generalized Markup Language), ODA(Office Document Architecture), DAP(Document Application Profile), Abstract Syntax Notation Ope Syntax Notation One.

The Office Systems Engineering Group (OSE) at the National Institute of Standards and Technology (NIST) was tasked by the Computer-aided Acquisition and Lo gistic Support (CALS') Project Office to bring CALS' requirements to the Open Systems Interconnection requirements to the Open Systems Interconnection (OSI) Implementor's Workshop sponsored by NIST. CALS tasked the OSE Group to assist in the SGML encoding of the Office Document Architecture (ODA) Document Application Profile (DAP). NIST offered to encode the ODA DAP in the Standard Generalized Markup Language (SGML) to illustrate the similarities between the two standards and to provide a common SGML/ASN.1 profile. The report describes in various levels of detail the two international standards. It then levels or detail the two international standards. It their discusses, by offering a simple example, the methodology involved in performing an SGML encoding. Subsequently, it examines the SGML encoding of the ODA DAP. The report provides two accompanying tables with the SGML encoding and finishes with a brief summer of the two standards. mary of the two standards.

101,346 PB91-187708 PC A06/MF A01 National Inst. of Standards and Technology (CSL), Gaithersburg, MD.
Tiled Raster Graphics and MIL-R-28002A: A Tutori-

F. E. Spielman, and L. H. Sharpe. Apr 91, 106p NISTIR-4567

Sponsored by Assistant Secretary of Defense (Production and Logistics), Washington, DC. Computer-Aided Acquisition and Logistic Support Program.

Keywords: \*Computer graphics, \*Sweep generators, Standards, Documents, Standardization, Image processing, Data compression, Coding, Software tools, \*Military specification MIL-R-28002A, Abstract Syntax Notation One, Computer-aided Acquisition and Logistic Support. tic Support.

The report examines the technical issues facing an implementor of the raster data interchange format defined in military specification MIL-R-28002A. Information previously scattered throughout several standards is incorporated into the report for ease of reference. The National Institute of Standards and Technology Office Document Architecture Raster Document Application Profile (NIST ODA Raster DAP) is analyzed with regard to both notation and intent.

PB91-193821 PC A03/MF A01 National Inst. of Standards and Technology (CSL), Gaithersburg, MD. NIST Support of the CALS Program: 1990 Synop-

S. J. Kemmerer. Jun 91, 22p NISTIR-4609

Keywords: \*Project management, Data transmission, Computer graphics, Documents, Standards, Administration, Data management, Computer security, Tele-communication, Bibliographies, \*CALS(Computer-aided Acquisition and Logistics Support), \*NIST(National Institute of Standards and Technolo-

The report summarizes overall Computer-aided Acquisition and Logistics Support (CALS) program management, technical support, and administration provided by National Institute of Standards and Technology (NIST). A brief summary of some of the 1990 activities is offered in each of the general technical support areas: electronic data interchange, graphics, docu-ment standards, raster compression, data management, security, and data communication. Most of the NIST deliverables given to the CALS Office have since been published for easier access by the CALS community. The report offers the titles and brief abstracts of such published deliverables, as well as titles and abstracts for those NIST CALS deliverables published in previous years.

101,348 PB91-194506 PC A14/MF A02 National Inst. of Standards and Technology (CSL), Gaithersburg, MD.

NIST Support for the Computer-Aided Acquisition and Logistic Support (CALS) Program in the Area of Graphics Standards, Calendar Year 1990.

Rept. for Oct 89-Dec 90. D. R. Benigni. May 91, 311p NISTIR-4579 See\_also PB90-228016 and PB90-257759. Sponsored by Office of the Secretary of Defense, Washington, DC.

Keywords: \*Logistics support, \*Computer applica-tions, \*Computer graphics, \*Standards, Require-ments, Federal information processing standards, Specifications, Software tools, CALS(Computer-aided Acquisition and Logistic Support), NIST(National Institute of Standards and Technology), Department of De-

Computer-aided Acquisition and Logistic Support (CALS) is a program of the Office of the Secretary of Defense. Its objective is to establish an integrated set of standards and specifications for the creation, management, and exchange of logistics data and product development data-including graphical data-by computer. Since FY86, the National Institute of Standards and Technology (NIST) has been funded to recommend the standards to satisfy CALS requirements for system integration and digital data transfer, and to accelerate standards implementation. The report comprises the continuing work of the NIST Graphics Software Group in support of the CALS Program for 1990. The format of the report combines the separate task deliverables assigned to the NIST Graphics Software Group for 1990, which were as follows: (1) update Computer Graphics Metafile (CGM) Application Profile; (1) injury to the task of the computer Graphics Metafile (CGM) Application Profile; (2) inject CALS requirements into the standards committees' work on Amendments to the CGM standard; (3) produce a software tool to determine conformance of a metafile to the CGM standard and to MIL-D-28003; and (4) explore potential sources of generator and interpreter conformance test capabilities.

101,349 PB92-112440 PC A99/MF A06 National Inst. of Standards and Technology (CAML), National first. Or Standards and Technology (CAME), Gaithersburg, MD. Office of Applied Economics. Economic Analysis for Military Construction (MILCON) Design. Concepts, Techniques, and Ap-plications for the Analyst. Instructor's Manual. R. T. Ruegg, and S. K. Fuller. Sep 91, 637p NISTIR-90/4256

See also Student's manual, PB92-112457. Sponsored by Corps of Engineers, Huntsville, AL. Huntsville Train-

Keywords: \*Military training, \*Construction management, \*Economic analysis, \*Instructors, Benefit cost analysis, Energy conservation, Life cycle costs, Structural design, Manuals, Requirements, Buildings, Military facilities, Case studies.

The Instructor's Manual is a detailed guidebook for teaching the five-day course, 'Economic Analysis for Military Construction Design: Concepts, Techniques, and Applications for the Analyst'. It provides numerous aids for teaching the course, including pre-course check-lists, descriptions of instructional techniques, tips for making the course more effective, and step-bystep lesson plans. Copies of all slides and vugraphs are reproduced in the guidebook, together with presentation text, exercises, and solutions. Through special fonts and a page numbering system geared to the Student Manual, the instructor always knows exactly what the student sees without the necessity of manipulating both manuals at once.

101,350

PB92-112457 PC A21/MF A04 National Inst. of Standards and Technology (CAML), Gaithersburg, MD. Office of Applied Economics.
Economic Analysis for Military Construction (MILCON) Design. Concepts, Techniques, and Applications for the Analyst. Student's Manual.

R. T. Ruegg, and S. K. Fuller. Sep 91, 476p NISTIR-90/4255

See also Instructor's manual, PB92-112440. Sponsored by Corps of Engineers, Huntsville, AL. Huntsville Training Div.

Keywords: \*Military training, \*Construction management, \*Economic analysis, \*Students, Benefit cost analysis, Energy conservation, Life cycle costs, Structural design, Requirements, Military facilities, Buildings, Case studies, Manuals.

The manual is the class workbook for a five-day course, Economic Analysis for Military Construction Design: Concepts, Techniques, and Applications for the Analyst'. The course equips design professionals to conduct, document, and review economic studies of building and facility design alternatives in accordance with Army and Air Force requirements. It demonstrates a variety of applications through realistic examples and case studies. The workbook covers 16 training modules; including orientation, pre and post tests, aids to learning, time value of money, mathematical oper-ations, general economic studies, energy conservation studies, data, computer software, and uncertainty and risk analysis. Each of the technical modules lists learning objectives and summarizes key points. The manual is designed not as a stand-alone tutorial, but as a working document for a course taught by an instructor who provides additional information.

# **NATURAL RESOURCES** & EARTH SCIENCES

# Cartography

101,351

PB91-147678 Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Mathematical Analysis Div. Non-Linear Contour-to-Grid Digital Interpolation.

Final rept.

B. A. Mandel. 1986, 9p

See also AD-A180 632.

Pub. in Proceedings of DOD Mapping, Charting, and Geodesy (MC&G) Conference, Alexandria, VA., May 8, 1986, 9p.

Keywords: \*Contours, \*Grids(Coordinates), \*Maps, \*Terrain models, Triangulation, Mapping, Conversion, Elevation, Interpolation, Methodology, Nonlinear systems, Digital systems, Sampling, Reprints.

A technical approach to the task of performing a contour-to-grid conversion using non-linear interpolation has been studied. The approach consists of reconstructing a terrain surface from the digitized contour lines on a map. The approximating surface is defined in terms of a partition of the region into irregular triangles obtained by a Voronoi method. The vertices of the gles obtained by a voluntification. The values of the triangles are selected by sampling a large set of digitized contour data with a tolerance band technique. The result is a smooth synthetic surface with which the elevation of any given point can be calculated. Therefore, grids of any given dimensions can be generated.

### **Forestry**

101,352
PB91-143305
PC A04/MF A01
National Inst. of Standards and Technology (NEL),
Gaithersburg, MD. Center for Fire Research.
Canadian Mass Fire Experiment, 1989.
Final rept.
J. G. Quintiere, Nov 90, 64p NISTIR-4444

J. G. Quintiere. Nov 90, 64p NISTIR-4444 Sponsored by Defense Nuclear Agency, Washington,

Keywords: \*Fire tests, \*Forest fires, \*Environmental impacts, \*Atmospheric motion, Combustion, Smoke, Particulates, Air pollution, Plumes, Fuel consumption, Clouds, Prescribed burning.

Working with Forestry Canada and the Ontario Ministry of Natural Resources, the Defense Nuclear agency carried out an extensively instrumented experiment of a prescribed burn in forest debris to simulate conditions of a mass fire. In addition to the Canadian team, a multi-institutional US team made both ground and airborne measurements of the fire and smoke conditions. The fire reported on was in Hill Township, Ontario and covered nearly 480 ha in its overall burning area. Both flaming and smoldering modes contributed to the energy and combustion products of the fire. Significant quantities measured and determined included estimations of energy release rate, emission factors for smoke particulates and species, ground level wind and temperatures, and aspects of cloud dynamics and cloud particles. The fire caused a capping cloud to form and reach a level of 6.5 km. Rain, snow, hail and lightning were reported along with ground level fire whirls and water spouts on the adjoining lakes. Fire spread rates reached 1 m/s and fire induced winds reached 12 m/s.

Geology & Geophysics

101,353
PB91-203026
Not available NTIS
National Inst. of Standards and Technology (NML),
Boulder, CO. Quantum Physics Div.
Lunar Laser Ranging.

Final rept. J. E. Faller, and J. O. Dickey. 1990, 2p Pub. in EOS 71, n21 p725-726, 22 May 90.

Keywords: \*Lunar rangefinding, \*Geodesy, Apollo 11 flight, Laser range finders, Earth rotation, Lunar landing, Gravitation, Reprints, Lunar libration, Nordvedt effect

At the 1990 AGU Spring Meeting in Baltimore, Md., on Tuesday morning, May 29, there will be the special joint Geodesy-Planetology session Apollo Lunar Laser Ranging and Our Lunar Return. The session of invited papers will focus on and, yes, celebrate lunar laser ranging, which has been made possible by simple laser reflectors of the type first left by Buzz Aldrin on the powdery surface of the Sea of Tranquility. The session has been arranged to recall that on July 20 of this past year we celebrated the twentieth anniversary of the first human landing on the Moon.

PB91-237396 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Gas and Particulate Science Div. Accelerator (14)C Dating of Late Pleistocene Me-

gafauna. Final rept.

T. Stafford. 1988, 3p Pub. in Current Research in the Pleistocene, v5 p41-43

Keywords: \*Radiocarbon dating, \*Age determination, \*Fossils, \*Geologic ages, Mass spectroscopy, Pleistocene epoch, Bones, Wildlife, Stratigraphy, Reprints.

A significant application of tandem accelerator mass spectrometry 14C dating has been attempting to resolve two, decades-old controversies---the timing of human migrations into the New World and the dating of Late Pleistocene megafaunal extinctions, which are nearly coincident with the Clovis-period hunters. The precise dating of the Clovis culture (Haunes 1984) has not been accomplished for the extinct, terminal Pleistocene faunas, which are dated to 10,000-12,000 yr

B.P. (Martin 1984) and into the Holocene (Kurten and Anderson 1980). Two questions remain to be resolved---are post 10,500 yr B.P. 14C dates accurate and what is the time range within which the genera became extinct. Direct dating of fossils is mandatory because the approach eliminates uncertainty from stratigraphic interpretation, bioturbation and sediment recycling. Although the problems with bone dating are longstanding (Taylor 1982; Ptorsch 1986; Stafford et al 1987), fossil bone can now be dated accurately if a rigorous biochemical and geochemical approach is taken (Stafford, Brendel and Duhamel 1988).

101,355
PB91-237404
Not available NTIS
National Inst. of Standards and Technology (NML),
Gaithersburg, MD. Gas and Particulate Science Div.
Accelerator Radiocarbon Dates on Charcoal, Shell,
and Human Bone from the Del Mar Site, California.
Final rept

T. W. Stafford, and R. A. Tyson. 1989, 7p Pub. in American Antiquity 54, n2 p389-395 1989.

Keywords: \*Radiocarbon dating, \*Age determination, \*Fossils, \*Site surveys, \*Geologic ages, California, Mass spectroscopy, Amino acids, Bones, Charcoal, Hemispherical shells, Reprints.

Accelerator radiocarbon dates on shell, charcoal, and human bone samples are an indication that human activity at the Del Mar site dates to 5000 yr B.P. and possibly from 7000 yr B.P. The shell and charcoal fragments were stratigraphically dislocated by extensive bioturbation and are evidence that accelerator dates on extremely small samples should be used with caution. Certain depositional environments will require multiple-dating within a site because single-sample dating will not yield definitive ages. Dating of individual amino acids from the Del Mar sphenoid yielded an average age of 4900 (+ or -) 40 yr and conclusively establishes the age for the Del Mar skull. The previously dated tibia was found to be contaminated with exogenous amino acids, thereby making its age uncertain.

**Mineral Industries** 

101,356
PB91-144337
PC A05/MF A01
Maryland Univ., College Park. Dept. of Mechanical Engineering

Investigation of Simulated Oil-Well Blowout Fires.
Annual rept.

J. P. Gore, S. M. Skinner, and U. S. Ip. Nov 90, 82p NIST/GCR-90/581 Grant NANB8D0834

Sponsored by National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Center for Fire Research.

Keywords: \*Blowouts, \*Oil wells, \*Fires, \*Fire protection, Heat flux, Temperature measurement, Flames, Fire extinguishers, Fire tests, Reaction kinetics, Burning rate.

A study of simulated oil well blowout fires aimed at improving predictive capabilities needed for the development of radiation and fire suppression technology is described. Measurements of temperature distributions and radiative heat flux to representative locations are used to evaluate the analysis. Methane/air flames with suppression and heptane+methane/air flames with suppression are considered. The analysis consists of (i) construction of state relationships for fuel with water addition and two phase fuel mixtures using species concentration data for single fuels with the help of mixing rules and (ii) application of an existing flow solver under the locally homogeneous flow approximation. The predictions and measurements are in reasonably good agreement. Direct verification of the mixing rule for state relationships and treatment of two phase flow effects is necessary for further improvement.

101,357
PB91-231597
PC A03/MF A01
National Inst. of Standards and Technology (NEL),
Gaithersburg, MD. Unmanned Systems Group.
Task Decomposition and Algorithm Development
for Real-Time Motion Control of a Continuous

Mining Machine. H. M. Huang, J. A. Horst, and R. Quintero. May 91, 46p NISTIR-4596

Sponsored by Bureau of Mines, Pittsburgh, PA.

Keywords: \*Mining equipment, \*Algorithms, \*Underground mining, \*Coal mining, \*Control systems design, Cutting, Real time operations, Systems engineering, Mining engineering, Error analysis, \*Continuous mining machines.

The drive toward increased safety for coal miners has led to the development of computer-assisted methods of underground coal mining. The development of control architectures and accompanying code for the control of the movement of continuous mining machines (tramming control) is an important part of this overall effort. The tramming control algorithm design described is in concert with hierarchical architecture design principles developed at National Institute of Standards and Technology (NIST), referred to as the Real-Time Control Systems (RCS) methodology. The algorithm design with accompanying code allows for the control of both cutting and free-space movement by a continuous mining machine (CM) and allows for a high degree of human operator interaction.

### Natural Resource Management

101,358
PB92-123116
PC A05/MF A01
Maryland Univ., College Park. Dept. of Fire Protection
Engineering.

Engineering.

Development of a Technique to Assess the Adequacy of the Municipal Water Supply for a Residential Sprinkler System.

dential Sprinkler System. J. A. Milke, and J. L. Bryan. Nov 91, 83p NBS/GCR-91/600

Grant NANB8D0814

See also PB88-155825. Sponsored by National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Center for Fire Research, and Fire Administration, Emmitsburg, MD.

Keywords: \*Assessments, \*Water supply, \*Municipalities, Residential buildings, Cost effectiveness, Water storage, Storage tanks, Plumbing, Prototypes, Water flow, Sprinklers, Piping systems, Evaluation.

The research effort developed a technique to assess the adequacy of the municipal water supply for residential sprinkler systems installed in one- and two-family dwellings. The effort is a continuation of a recently completed project which investigated cost-effective techniques for alleviation of deficiencies in the municipal water supply. In that effort, a need was identified to develop a technique to evaluate the adequacy of the municipal water supply. The report includes characterizing typical plumbing flow fixtures in residences to permit an analysis of the domestic water supply within a residence. Having characterized the residential flow devices, techniques to evaluate the domestic water supply are investigated. The investigation considers the feasibility of developing an inexpensive prototype apparatus with which to conduct the water supply evaluations.

### Soil Sciences

101,359

PB91-174680

Not available NTIS
National Inst. of Standards and Technology (NML),
Gaithersburg, MD. Gas and Particulate Science Div.
Wawayandaite, a New Calcium Manganese Beryllium Boron Sillicate from Franklin, New Jersey.
Final rept.

P. J. Dunn, D. R. Peacor, J. D. Grice, F. J. Wicks, and P. H. Chi. 1990, 4p Pub. in American Mineralogist 75, p405-408 1990.

Keywords: \*Nonmetalliferous minerals, \*Inorganic silicates, New Jersey, Crystal structure, Calcium compounds, Manganese compounds, Beryllium compounds, Boron compounds, Reprints, \*Wawayandaite.

Wawayandaite, a new mineral from Franklin, New Jersey, is found associated with willemite, friedelite, and numerous other minerals. It is monoclinic, space group P2/c or Pc, with a = 15.59(2), b = 4.78(1), c = 18.69(4) A, beta = 101.84(15) degrees, Z = 1. Chemical analyses yielded BeO 17.6, MgO 1.9, CaO 24.8, MnO 9.8, ZnO 1.1, B2O, 3.8, SiO2 28.2, H2O 9.6, Cl

# **NATURAL RESOURCES & EARTH SCIENCES**

### Soil Sciences

3.0, less O = Cl 0.7, total = 99.1 wt%. The idealized 3.0, less O = Cl 0.7, total = 99.1 wt%. The idealized chemical formula is Ca12Mn4B2Be18Si12O46(OH,Cl)30. Wawayandaite occurs as colorless platy crystals with a pearly luster; many are strongly curved. Cleavage is perfect on (010), D (sub measured) is approximateLy 3.0, D (sub calculated) = 2.98 g/cc. It is biaxial, negative, with 2V = 85 degrees alpha = 1.619, beta = 1.631, and qamma = 1.641.

Isotope ratio measurements in Mo and Sn by Sputter-Initiated Resonance Ionization Spectroscopy show that the response for odd isotopes and even isotopes can be dramatically different in some cases, even if the laser linewidth is larger than the span of the hyperfine structure and isotope shifts. Power broadening on the resonance transition has not removed the odd/even effect in the cases studied.

# NAVIGATION. **GUIDANCE**, & CONTROL

### **Navigation & Guidance System** Components

101,360 PB91-195354 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Robot Systems Div.
Real-Time Algorithms and Data Structures for Underwater Mapping.

Final rept.
D. N. Oskard, T. H. Hong, and C. A. Shafer. 1990, 7p
Pub. in IEEE (Institute of Electrical and Electronics Engineers) Transactions on Systems Man and Cybernetics 20, n6 p1469-1475 1990.

Keywords: \*Autonomous navigation, \*Mapping, Models, Underwater navigation, Data bases, Algorithms, Data structures, Real time systems, Hierarchies, Sonar detection, \*MAUV(Multiple Autonomous Underwater Vehicles).

As part of the Multiple Autonomous Underwater Vehicle (MAUV) project at the National Institute of Stand-ards and Technology, a spatial mapping system has been developed to provide a model of the underwater environment suitable for autonomous navigation. The system is comprised of multi-resolution depth maps designed to integrate sensor data with a priori model, an object/attribute database for storing information known about detected objects, and a set of flags to monitor abnormal or emergency conditions in the environment. The paper describes the organization and structure of the mapping system and the algorithms used to map terrain and obstacles detected by acoustic sonar.

# **NUCLEAR SCIENCE & TECHNOLOGY**

### Isotopes

101,361 PB92-116789 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Ionizing Radiation Div. Observation of Anomalous Isotope Ratios in SIRIS

Measurements of Molydenum. Final rept.

W. M. Fairbank, M. T. Spaar, J. E. Parks, and J. M.

Pub. in Proceedings of International Symposium on Resonance Ionization Spectroscopy and Its Applica-tions (4th), Gaithersburg, MD., April 10-15, 1988, p293-

Keywords: \*Molybdenum isotopes, \*Tin isotopes, \*Isotopes, Till isotopes, Till isotopes, State and State ture, Sputter-ion pumps, Reprints, Sputter-initiated resonance ionization spectroscopy.

### **Nuclear Instrumentation**

101.362 PB91-178855 PC A08/MF A01 National Inst. of Standards and Technology (NML), Gaithersburg, MD. Center for Radiation Research. Center for Radiation Research. 1990 Technical Activities.

C. E. Kuyatt. Feb 91, 158p NISTIR-4506 See also PB90-130279.

Keywords: \*Research projects, \*Radiation measuring instruments, \*Radiometric analysis, Methodology, Calibrating, US NIST, Tests, Radiation sources, Radiation dosage, Neutron fluence, \*NIST Center for Radiation dosage, Neutron fluence, \*NIST Center fluence, \*NIST Cent ation Research.

The report summarizes research projects, measurement method development, calibration and testing and data evaluation activities that were carried out during Fiscal Year 1990 in the NIST Center for Radiation Research. These activities fall in the areas of radiometric physics, radiation sources and instrumentation, and ionizing radiation.

101,363

PB92-116441 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Ionizing Radiation Div.

Effects of Absorbed Dose Rate, Irradiation Tem-

perature and Post-Irradiation Temperature on the Gamma Ray Response of Red Perspex Dosimeters.

Final rept

M. Al-Sheikhly, W. J. Chappas, W. L. McLaughlin, and J. C. Humphreys. 1991, 16p

Pub. in Proceedings of International Symposium on High Dose Dosimetry for Radiation Processing, Vienna, Austria, November 5-9, 1990, p419-434 1991.

Keywords: \*Radiation curing, \*Dosimeters, Gamma rays, Irradiation, Plastics, Calibrating, Temperature dependence, PMMA, Dyes, Color centers, Measurement, Reprints, Adsorbed dose, Radiochromic dosimeters.

The influences of irradiation temperature and gamma radiation dose rate on the response of red 4034 Perspex dosimeters have been reported in the literature to be of relatively minor consequence, particularly for irradiations at up to a temperature of 40 C and at absorbed dose rates of the order of 7 kGy/h (about 2Gy/s). The present study shows this to be true; however, if there are marked differences in the temperature (22 C to 50 C) during extended storage periods (up to 16 hours) after irradiation, there is a tendency to overestimate an unknown dose administered at the elevated temperature, as a result of using a calibration made at an ambient lower temperature (e.g. 22 C). The present study of dose rate effects also shows that there is a pronounced tendency to overestimate an unknown gamma ray dose administered at a relatively low dose rate (3 and 7 kGy/h) as a result of using a calibration made at a considerably higher dose rate (e.g. 31 kGy/ h), even when the temperature of irradiation and storage is controlled at 22 C.

101,364

398 1991.

PB92-116961 Not available NTIS National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Polymers Div. Radiochromic Film Dosimeter for Gamma Radi-

ation in the Absorbed-Dose Range 0.1 - 10 kGY. Final rent

H. M. Khan, M. Farahani, and W. L. McLaughlin. 1991, 4p Pub. in Radiation Physics and Chemistry 38, n4 p395-

Keywords: \*Film dosimetry, \*Gamma dosimetry, Food irradiation, Gamma rays, Dose-response relationships, Spectrophotometry, Reprints, \*Radiochromic film.

A commercially available leuco-dye film (FWT-63-02), having a thickness of 0.55 mm, has been investigated spectrophotometrically for its characteristics as a radiochromic dosimeter and for its potential use in food-irradiation applications. The gamma-ray irradiation of the nearly colorless, transparent film induces blue color with an absorption maximum at 600 nm. The increase in absorbance at 600 nm per unit thickness of film is linear with dose in the dose range up to 8 kGy, with a slope of 0.91/mm/kGy. After a modest additional increase during the first day following irradiation, the radiation-induced color is stable when stored at room temperature at least for 5 weeks. The response slope is 16% higher when stored at 60 C, however, after the initial 1-day increase it is stable for several weeks when stored at that temperature. The response of the dosimeter is independent of dose rate in the range 0.5-170 Gy/min.

101.365

PB92-117100 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Ionizing Radiation Div. Dosimetry: New Approaches for New Challenges.

W. L. McLaughlin. 1991, 31p Pub. in Proceedings of Nordion Gamma Processing Seminar (4th), Ottawa, Ontario, Canada, May 26-31, 1991, p1-31.

Keywords: \*Dosimetry, \*Radiation curing, \*Chemical radiation effects, \*Plastics, Polymeric films, Gamma rays, PMMA, Polymers, Quality control, Mapping, Dosimeters, Dichromates, Photographic film dosimeters, Reprints, Adsorbed dose, Radiochromic dosimeters.

During the past few years, since the time of the 3rd Gamma-Processing Seminar in 1983, new and improved dosimetry systems and applications have been introduced for radiation processing. These include better reference and transfer standards; more accurate calculations. (FSR parallysis) with creatures. rate calorimeters; alanine (ESR analysis) with greater precision and wider dose ranges; several liquid dosimeters (UV and visible spectrophotometry), and radiochromic dye organic solutions; several solid polymeric dosimeters, including new polymethylmethacrylate (Perspex) and Nylon and other plastic films. The latter systems are commercially available in large quantities, and are relatively inexpensive and easy to use over the absorbed dose ranges encountered in radiation processing (10-10 to the 5th power Gy). Some of these are especially useful for dose mapping in radiation processed products, as a means of determining the locations and mean values of minimum and maximum doses and the dose uniformity ratios, and others are used for day-to-day quality control measurements.

101,366

Not available NTIS PB92-117126 National Inst. of Standards and Technology (NML), Gaithersburg, MD. Ionizing Radiation Div. 2-Deoxy-D-Ribose Aqueous Solution as a Gamma-

Ray Dosimeter.

Final rept. W. L. McLaughlin, M. Farahani, and J. H. Liang.

1991, 13p Pub. in Proceedings of International Symposium on High Dose Dosimetry for Radiation Processing, Vienna, Austria, November 5-9, 1990, p159-171 1991.

Keywords: \*Dosimeters, \*Gamma rays, \*Deoxyribose, \*Arabinose, Optical activity, Aqueous solutions, Irradiation, Chemical radiation effects, Radiation curing, Polymers, Maltose, Storage life, Time dependence, Temperature dependence, Saccharides, Sugars, Resister

The change in the angle of optical rotation (delta alpha) of buffered aqueous solution (pH7) of 2-deoxy-D-ribose due to irradiation with gamma radiation gives a convenient means of dosimetry. The method is shown to be suitable with solutions stored and irradiated in sealed glass ampoules. The dosimeter solution is not sensitive to light and is not affected by contamination by trace organic or inorganic impurities. The radiation induced value of (delta alpha) is reproducible to within + or - 3% (95% confidence level) at dose levels of 50-500 kGy. The useful radiation response range of the dosimeter is 10 to 1000 kGy, and this represents a more sensitive and reproducible response than the conventional optical rotation of glucose or sucrose so-lution. Comparisons were also made with solutions of D-(-) arabinose and D-(+)-maltose. The value of (delta alpha) of 2-deoxy-D-ribose does not change during storage and reading, over at least several weeks stor-

# **Nuclear Instrumentation**

age period. There is no appreciable variation of response with dose rate, but the irradiation temperature coefficient over the temperature range 0 to 17 C is approximately + 1.5% C, and at higher temperatures up to 33 C is + 3.0% C.

### Radioactive Wastes & Radioactivity

101,367

NUREG/CR-5711 PC A06/MF A02 National Inst. of Standards and Technology, Gaithersburg, MD.

Assessment of Uncertainties in Measurement of pH in Hostile Environments Characteristic of Nuclear Repositories.

Technical rept. 30 Jun 87-28 Feb 91.

K. G. Kreider, M. J. Tarlov, and P. H. Huang. Oct 91, 102p

Also available from Supt. of Docs. See also NUREG/ CR-5166 and NUREG/CR-5484. Sponsored by Nuclear Regulatory Commission, Washington, DC. Div. of Engineering.

Keywords: \*Electrodes, \*Radioactive wastes, \*pH, \*Thin films, Iridium oxides, Data covariances, Tuff, Measurement, Corrosion resistance, Aqueous solu-tions, Ceramics, Sputtering, Spectrum analysis, Electrochemistry, High temperature tests.

The report focuses on evaluation and characteristics of sputtered thin film pH electrodes which can be used to assess the corrosivity of hot (100 C) aqueous solutions present in nuclear repositories. Sputtered thin tions present in nuclear repositories. Sputtered thin films have the advantages of high temperature capability, ruggedness, and low cost. The sputtered iridium oxide films (SIROF) were found to have a linear, 58 mV/pH, response to changes in pH. They had little hysteresis but drifted approximately 0.2 V over a period of two days exposure to pH 2-12 solutions. The films were found to be insensitive to interference from most ions such as alkali ions but had redox sensitivity to ferri-/ferrocyanide ions. Although special surface treatments were needed for the films for good adherence at 200 C the films were not degraded after 20 hours exposure at pH 4, 7, and 10 at 200 C. Ruthenium oxide sputtered films performed equally well to the irid-ium oxide films in parallel tests. The report also contains information on electrochemistry and testing of thin film electrodes and the characterization of the thin films by x-ray photoemission spectroscopy, ultraviolet photoemission spectroscopy, and ion scattering spectroscopy.

101,368

NUREG/CR-5716 PC A05/MF A01 Arizona Univ., Tucson. Dept. of Soil and Water Sci-

Model Validation at the Las Cruces Trench Site.

Technical rept. 1 Nov 90-20 May 91. R. G. Hills, and P. J. Wierenga. Jun 91, 94p

Also available from Supt. of Docs. Prepared in cooperation with New Mexico State Univ., Las Cruces. Dept. of Mechanical Engineering. Sponsored by Nuclear Regulatory Commission, Washington, DC. Div. of Engineering.

Keywords: \*Radioactive waste facilities, \*Low level radioactive wastes, Field tests, Water flow, Radionuclide migration, Soils, Ground disposal, Las Cruces Trench

A series of dynamic field experiments have been performed at the Las Cruces Trench Site to provide data to test deterministic and stochastic models for water flow and solute transport in spatially variable unsaturated soils. Two experiments were performed to provide support for model validation efforts during Phase I of INTRAVAL (an international effort towards validation of geosphere models for transport of radionuclides) and a third experiment is currently underway to support the INTRAVAL Phase II efforts. The third experiment utilized different boundary and initial conditions and additional chemical tracers. The report summarizes the Las Cruces Trench Site model validation efforts and presents the INTRAVAL Phase II validation plans. The Phase II validation strategy is discussed in detail

### Reactor Engineering & Nuclear Power **Plants**

101 369 PB91-222687 PC A10/MF A03 National Inst. of Standards and Technology (EEEL), Gaithersburg, MD. Electricity Div. Annotated Bibliography: Diagnostic Methods and

Measurement Approaches to Detect Incipient De-

fects Due to Aging of Cables.
F. D. Martzloff, and A. G. Perrey. Jul 91, 224p NISTIR-4485

Sponsored by Nuclear Regulatory Commission, Washington, DC.

Keywords: \*Bibliographies, \*Defects, \*Nuclear power plants, \*Cables, \*Nondestructive tests, Surveys, Cable insulation, Wire, Detection, Aging, Damage assess-

Open-literature papers and some limited-distribution documents were reviewed in a search to identify promising approaches to the in-situ detection of incipient defects in nuclear power-plant cables. The search was extended to the topics of detection of any defect, to radiation effects, and to basic considerations on partial discharges. The report presents a review of 150 papers that appeared significant on the basis of their title, but many of which were found not applicable upon close review. A compilation of 850 references cited in the reviewed papers is included in the report.

PB92-123074 PC A04/MF A01 National Inst. of Standards and Technology, Gaithersburg, MD.

Fire-Plume-Generated Ceiling Jet Characteristics and Convective Heat Transfer to Ceiling and Wall Surfaces in a Two-Layer Zone-Type Fire Environment: Uniform Temperature Ceiling and Walls. L. Y. Cooper. Nov 91, 58p NISTIR-4705

Sponsored by Nuclear Regulatory Commission, Washington, DC.

Keywords: \*Fires, \*Heat transfer, \*Reactor safety, \*Walls, \*Ceilings(Architecture), Subroutines, Mathematical models, Algorithms, Computer programs, Temperature distribution, Jet flow, Heat flux, Plumes, Velocity, CEILHT Subroutine.

The work presents a model to predict the instantaneous rate of convective heat transfer from fire plume gases to the overhead ceiling surface in a room of fire origin. The room is assumed to be a rectangular parallelopiped and, at times of interest, ceiling temperatures are simulated as being uniform. Also presented is an estimate of the convective heat-transfer, due to ceiling-jet-driven wall flows, to both the upper and lower portions of the walls. The effect on the heat transfer of the location of the fire within the room is taken into account. Finally presented is a model of the velocity and temperature distributions in the ceiling jet. The model equations were used to develop an algorithm and associated modular computer subroutine to carry out the indicated heat transfer calculations. The subroutine is written in FORTRAN 77 and called CEILHT. The algorithm and subroutine are suitable for use in two-layer zone-type compartment fire model computer codes.

PC A05/MF A01 PB92-126598 National Inst. of Standards and Technology (BFRL), Gaithersburg, MD.

Predicting the Remaining Service Life of Concrete.
J. R. Clifton. Nov 91, 84p NISTIR-4712
See also PB89-215362 and PB91-107219. Prepared in

cooperation with Oak Ridge National Lab., TN., and Nuclear Regulatory Commission, Washington, DC.

Keywords: \*Nuclear power plants, \*Service life, \*Conretes, Performance, Estimates, Comparisons, Accelerated tests, Statistical models, Mathematical models, Degradation, Corrosion, Sulfates, Alkali-aggregate reactions, Frost, Leaching, Radiation.

The report examines the basis for predicting the remaining service lives of concrete materials of nuclear power facilities. Methods for predicting the service life of new and in-service concrete materials are analyzed. These methods include (1) estimates based on experience, (2) comparison of performance, (3) accelerated testing, (4) stochastic methods, and (5) mathematical modeling. New approaches for predicting the remaining service lives of concrete materials are proposed and recommendations for their further development are given. Degradation processes are discussed based on considerations of their mechanisms, likeli-hood of occurrence, manifestations, and detection. They include corrosion, sulfate attack, alkali-aggregate reactions, frost attack, leaching, radiation, salt crystallization, and microbiological attack.

### Reactor Fuels & Fuel Processing

101 372

PB91-158733 Not available NTIS National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Metallurgy Div.

Corrosion Behavior of Zirconium Alloy Nuclear

Fuel Cladding.

Final rept.

A. C. Fraker, and J. Harris. 1990, 8p Sponsored by Nuclear Regulatory Commission, Washington, DC. Office of Nuclear Material Safety and Safe-

guards. Pub. in Materials Research Society Symposium Proceedings, v176 p549-556 1990.

Keywords: \*Zircaloys, \*Corrosion tests, \*Nuclear fuel claddings, Passivity, Polarization, Crevice corrosion, Surface finishing, Electrical faults, Chemical radiation effects, Alkalinity, Temperature dependence, Reprints.

Zircalov-2 and -4 are used as nuclear fuel cladding. Both alloys are more than ninety-eight percent zirconium and are corrosion resistant to various media. Electrochemical measurements using polarization techniques have been made on these alloys in aqueous media with a pH of 8.5 and varying ionic concentration (1X and 10X) at temperatures of 22C and 95C. Results showed that under the test conditions of the study these alloys passivated and had negligible corrosion rates, but there were some variations in passivation due to surface preparation and some crevice corrosion was observed. Data are presented and discussed in terms of passivity, breakdown potential and susceptibility to localized corrosion.

# **Reactor Materials**

101.373

PR91-189316 Not available NTIS National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Metallurgy Div. Plastic Zone Formation Around an Arresting

Crack. Final rept.

R. J. Fields, and R. deWit. 1990, 8p

Sponsored by Nuclear Regulatory Commission, Washington, DC.

Pub. in International Jnl. of Fracture 42, n3 p231-238 1990.

Keywords: \*Crack arrest, \*Pressure vessels, \*Reactor materials, \*Steels, \*Fracture mechanics, \*Strain tests, Plasticity, Strain gages, Reactor components, Velocity, Reprints.

The evolution of strain near the tip of an arresting cleavage crack was followed using a strain gage technique. The results were obtained in a body so large that reflected elastic waves did not contribute significantly to the strain records during the time interval of interest. The measurements were made using a linear array of strain gages located along the intended crack path and 0.65B (B = specimen thickness) above this plane. The gages were read using instrumentation capable of resolving strain in time intervals of less than 10 microseconds. To within the resolution of the technicque, the results did not suggest plasticity near the rapidly propagating, cleavage crack tip. At the instant of arrest, however, the strain gages detected a plastic zone which increased in intensity over a period of several milliseconds. This increasing intensity was interpreted as an elastic-plastic boundary emanating from the arresting crack tip and eventually reaching an equi-librium size, i.e., that predicted from the applied stress intensity factor and the static plastic properties. A simple analysis is presented to estimate the velocity of

### **NUCLEAR SCIENCE & TECHNOLOGY**

### **Reactor Materials**

the elastic-plastic boundary from the strain data and results are given for several experiments.

# **OCEAN TECHNOLOGY & ENGINEERING**

# Biological Oceanography

PB91-184796 PC A03/MF A01 National Inst. of Standards and Technology (CSTL),

National Inst. of Standards and recurringly (65.2), Gaithersburg, MD. Alaska Marine Mammal Tissue Archival Project: Revised Collection Protocol.
P. R. Becker, S. A. Wise, B. J. Koster, and R. Zeisler. Mar 91, 409 NISTIR-4529
Prepared in cooperation with National Ocean Service, Anchorage, AK. Arctic Environmental Assessment Center. Sponsored by Minerals Management Service, Anchorage. AK. Alaska Outer Continental Shelf Office.

keywords: \*Alaska, \*Aquatic animals, \*Mammals, Tissues(Biology), Archives, Sampling, Procedures, Kevwords:

In 1987, the Outer Continental Shelf Studies Program of the Minerals Management Service (MMS) provided funds to the Ocean Assessments Division (OAD) Alaska Office, National Oceanic and Atmospheric Administration (NOAA), to establish and conduct a program of collecting tissues from Alaska marine mam-mals and storing them under conditions which would allow for future analyses for substances indicative of contamination from offshore oil and gas, and mining activities. Cataloging and archiving of samples are conducted at the Alaska Marine Mammal Tissue Archive, which is maintained by NIST in its National Biomonitoring Specimen Bank (NBSB), Gaithersburg, Maryland. The report presents the protocol used in the collection and archival process.

# Marine Engineering

Final rept.

PB91-158782 Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Robot Systems Div.
Real-Time Hierarchical Planning for Multiple Mobile Robots.

M. Herman, and J. S. Albus. 1987, 10p Pub. in Proceedings of DARPA Knowledge-Based Planning Workshop, Austin, TX., December 8-10, 1987, p22-1-22-10.

Keywords: \*Underwater vehicles, \*Robotics, Control systems, Real time, Knowledge bases(Artificial intelligence), Reprints, MAUV(Multiple Autonomous Underwater Vehicles), Hierarchical control.

Multipule Autonomous Underwater Vehicles (MAUV) project is described. The goal of the project is to have multiple underwater vehicles exhibiting intelligent, autonomous, cooperative behavior. The MAUV control system is hierarchically structured and incorporates sensing, world modeling, planning and execu-tion. The levels in the hierarchy include a mission level, a group level, a vehicle task level, and an elemental action level. Issues of realtime planning and dynamic replanning in unstructured environments are discussed.

101,376 PB92-108935 PC A05/MF A01 National Inst. of Standards and Technology (BFRL), Gaithersburg, MD.
Navy Safety Center Data on the Effects of Fire Pro-

tection Systems on Electrical Equipment.

R. S. Levine. Apr 91, 86p NISTIR-4620
Portions of this document are not fully legible. Sponsored by Nuclear Regulatory Commission, Washington, DC

Keywords: \*Fire protection, \*Electrical equipment, \*Fire damage, \*Fire extinguishing agents, \*Shipboard fire control, Fire extinguishers, Sprinkler systems, Safety engineering, Fire hazards, Accident records, Tables(Data), Fire detection systems, Naval ships, Submarines, Halon, Carbon dioxide, Military facilities, Accident statistics.

Records of the Navy Safety Center, Norfolk, VA were reviewed to find data relevant to inadvertant operation of installed Fire Extinguishing Systems in civilian Nu-clear power plants. Navy data show the incidence of collateral fire or other damage by fresh water on oper-ating electrical equipment in submarines, and in shore facilities is about the same as the civilian experience, about 30%. Aboard surface ships, however, the collateral damage incidence is much lower, about 15%. With sea water, the collateral damage incidence is at least 75%. It is concluded that the fire extinguisher water has to be contaminated, as by rust in sprinkler systems or deposited salt spray, for most collateral damage to occur. Reasons for inadvertant operation (or advertant operation) of firex systems at shore facilities, submarines, and surface ships resemble those for nuclear power plants. Mechanical or electrical failures lead the list, followed by mishaps during maintenance. Detector and alarm system failures are significant problems at navy shore facilities, and significant at nuclear power plants. Fixed halon and CO2 systems in shore facilities cause no collateral damage. Lists of in-dividual Navy incidents with water and with halon and carbon dioxide are included as appendices to the

# Physical & Chemical Oceanography

101,377 PB91-149237 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Organic Analytical Research Div.
Preparation and Analysis of a Marine Sediment
Reference Material for the Determination of Trace Organic Constituents.

Final rept. M. M. Schantz, B. A. Benner, S. N. Chesler, B. J. Koster, and K. E. Hehn. 1990, 14p Pub. in Fresenius Jnl. of Analytical Chemistry 338, p501-514 1990.

\*Marine \*Sediments, Keywords: environments, Standards, \*Aromatic polycyclic hydrocarbons, \*Polychlorobiphenyl compounds, Liquid chromatography, Gas chromatography, Mass spectroscopy, Trace ele-ments, Sulfur, Contaminants, Reprints, Standard reference materials.

A new marine sediment Standard Reference Material (SRM) has been prepared and analyzed for the determination of trace organic constituents. SRM 1941. Organics in Marine Sediment, has been certified for concentrations of 11 PAHs using results obtained from gas chromatography (GC) with flame ionization detections. tion, gas chromatography-mass spectrometry, and liquid chromatography with fluorescence detection. Non-certified values for 24 additional PAHs are also reported. GC with electron capture detection was used to provide non-certified concentrations for 15 PCB cogeners and 7 chlorinated pesticides. In addition to the organic contaminants, concentrations of 32 major and trace elements were determined using neutron activation analysis, and the sulfur content was also determined using isotope dilution thermal ionization mass spectrometry.

# ORDNANCE

### Ammunition, Explosives, & **Pyrotechnics**

101,378 PB92-116292 PC A09/MF A02 National Inst. of Standards and Technology (EEEL), Boulder, CO. Electromagnetic Fields Div. Quantifying Standard Performance of Electromagnetic-Based Mine Detectors.

W. L. Gans, R. G. Geyer, and W. K. Klemperer. Oct 91, 180p NISTIR-3982

See also AD-A226 626. Sponsored by Army Belvoir Research Development and Engineering Center, Fort Belvoir, VA:

Keywords: \*Mine detectors, Buried objects, Dielectric properties, Portable equipment, Electromagnetic properties, Soil properties, Remote sensing, Basic programming language, Computer programs, Permeability, Permittivity, Sensitivity, Algorithms.

This is a final report to sponsor on work performed by National Institute of Standards and Technology (NIST) personnel from January 1, 1985 to December 31, 1990. An overview of the theory of the electromagnetic properties of soils is presented along with a brief review of existing technologies for the detection of buried objects using electromagnetics. The critical electromagnetic performance factors for portable EM mine detectors that NIST has identified are presented, along with a discussion of measurement systems for measuring the constitutive properties of soil and minelike materials. Recommendations are then presented for a measurement system configuration that should meet most of the Army's requirements. A recommended mine detector testing strategy is then presented along with a set of instructions for specific tests and an algorithm for comparatively scoring the performance of detectors. The tests and the scoring algorithm are as specific and as detailed as is possible at this stage of development. Last, a section is included that contains NIST's recommendations for the test data that should be archived.

# **Combat Vehicles**

101,379

PB91-134726 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Robot Systems Div.

Control System Architecture for Unmanned Ground Vehicles.

Final rept.

S. Szabo, H. Scott, and R. Kilmer. 1990, 9p Pub. in Proceedings of AUVS-90 Technical Symposium, Dayton, OH., July 30-August 1, 1990, p258-266.

\*Ground vehicles, \*Military vehicles, Kevwords: Remote control, Artificial intelligence, Systems engineering, Reprints, \*Antonomous control, Teleoperation, Robotics, Control systems, Real time systems, National Institute of Standards and Technology.

The U.S. Army Laboratory Command is spearheading a program designed to demonstrate cooperative real-time control of multiple unmanned ground vehicles. The program, titled TEAM, involves the teleoperated control of two vehicles from remotely located operator control stations. The function of the system is to provide remote operation of military vehicles equipped with any of a variety of reconnaissance or related mission packages. The National Institute of Standards and Technology's (NIST's) role in the program is to apply their hierarchically-structured real-time sensorbased control architecture, originally developed for the control of industrial robots, to the design of the supervisory control systems in the two vehicles and the operator control stations. The paper presents a description of the NIST Real-time Control System (RCS) architecture for the TEAM program. A general description of the TEAM operational scenarios and functional requirements relevant to these control systems is provided. The overall control architecture developed on the basis of these requirements is presented.

# PHOTOGRAPHY & RECORDING DEVICES

# **PHYSICS**

# **Recording Devices**

101,380 PB91-132258 PC A03/MF A01 National Inst. of Standards and Technology, Gaithersburg, MD.

Overview of the Product Data HyperStandard CD-**ROM Prototype.** 

S. Ressler. Nov 90, 16p NISTIR-4470

Keywords: \*Information systems, \*Information retriev-Standardization, Specifications, Prototypes, Data al, \*Standardization, Specifications, Prototypes, Data storage devices, Cost effectiveness, Computer systems hardware, \*CD ROM, \*Product data exchange, \*Product Data HyperStandard CD ROM, STEP(Standard for the Exchange of Product Model Data), PDES(Product Data Exchange using STEP), CALS(Computer aided Acquisition and Logistics Support), Computer aided design.

The paper describes the contents of the Product Data HyperStandard CD-ROM Prototype containing information related to product data standards. HyperStandard is a generic term describing the application of hy-pertext and multimedia technologies to standards in general. The CD-ROM contains both browsers for perusing the documents, and a number of other items of interest to the product data community. These include: IGES Version 5; the CALS specifications; preliminary STEP drafts, PDES, Inc. technical documents; the NIST PDES Toolkit; plus miscellaneous other pieces of information. (The sources of data for the document browsers on the CD-ROM prototype were the original electronic documents used to print those documents.) All of these data combined should serve as a useful repository of information for the community of technical experts developing product data standards. This variety of information has been assembled to demonstrate the community of the community strate that CD-ROM's are a convenient and cost-effective medium for use by the people involved in product data standardization efforts.

101,381 PB92-126549 PB92-126549 PC A04/MF A01 National Inst. of Standards and Technology (CSL),

Raithersburg, MD.

3480 Type Tape Cartridge: Potential Data Storage Risks, and Care and Handling Procedures to Minimize Risks.

Final rept.

M. P. Williamson. Nov 91, 60p NIST/SP-500/199 Also available from Supt. of Docs. See also PB83-237271 and PB88-233135. Sponsored by National Environmental Satellite, Data, and Information Service, Washington, DC.

Keywords: \*Data storage devices, \*Computer storage devices, \*Magnetic tapes, CLASS 3480 cartridge tape system, Magnetic tape cartridges.

The 3480 type media was introduced to the data storage industry in 1984. Early problems were reported due to premature degradation of the polyester polyure-thane binder. In addition, the lack of guidelines for proper care and handling increased the risks associated with the strategy of date to the 200 here again. ed with the storage of data on the 3480 type media. After approximately seven years experience, media manufacturers have significantly improved their binder manulacturers have significantly improved their binder formulations. Furthermore, 3480 type media users from government and industry have experienced the dependability and, conversely, the problems associated with the storage of data on the 3480 type media. The National Institute of Standards and Technology (NIST), under the sponsorship of the National Oceanic and Atmospheric Administration (NOAA), has undertaken an experience of the sectorical risks associated. and Affinisher Administration (ROAA), has different administration taken an appraisal of the potential risks associated with the storage of data on the 3480 type media. In addition, the study summarizes reasonable procedures for the care and handling of the 3480 type media in order to minimize potential risks. The conclusions of the NIST study are based on information gathered by NIST from pertinent scientific literature, and interviews with 3480 type technology users and manufacturers.

### **Acoustics**

101.382 Not available NTIS PB92-116847 National Inst. of Standards and Technology (NML), Gaithersburg, MD. Thermophysics Div. Accurate Acoustic Measurements in Gases Under

Difficult Conditions.

Final rept.

K. A. Gillis, M. R. Moldover, and A. R. H. Goodwin. 1991, 5p

Sponsored by Department of Energy, Washington, DC., and Department of the Navy, Washington, DC. Pub. in Review of Scientific Instruments 62, n9 p2213-2217 Sep 91.

Keywords: \*Test equipment, \*Waveguides, \*Sound waves, \*Gases, \*Acoustics, Measurement, Diaphragms(Mechanics), Transducers, Resonators,

Accurate measurements of the speed of sound in gases are often made using metal resonators with small transducers that perturb the resonance frequencies in minor and predictable ways. The method is extended to gases that may be corrosive and to high temperatures by using remote transducers coupled to a resonator by acoustic waveguides. Thin metal diaphragms separate the waveguides from the resonator. Thus, only metal parts come into contact with the test gas. In the present apparatus, any gas compatible with gold and stainless steel can be studied.

101.383 PB92-117456 Not available NTIS National Inst. of Standards and Technology (EEEL), Boulder, CO. Electromagnetic Fields Div.

Probe-Corrected Spherical Near-Field Scanning

Theory in Acoustics.

Final rept.

Pub. in Proceedings of IEEE (Institute for Electrical and Electronics Engineers) Instrumentation and Measurement Technology Conference Enhancing Productivity with Instrumentation and Measurement Technologies, Atlanta, GA., May 14-16, 1991, p283-286.

Keywords: \*Acoustic fields, \*Sound transducers \*Transducers, Acoustic measurement, Spherical waves, Near field, Scanning, Probes, Reprints.

Spherical near-field scanning is well known in electro-magnetics. The acoustical analog is outlined here. Data are taken, with an arbitrary probe, on a spherical surface surrounding an unknown transducer. The algorithms uses these data to characterize the fields of the transducer everywhere outside the measurement sphere. The results can be corrected for probe effects if the probe's receiving pattern is known.

# Fluid Mechanics

DE91012660 PC A03/MF A01 National Inst. of Standards and Technology, Boulder, CO. Thermodynamics Div.

Integrated theoretical and experimental study of the thermophysical properties of fluid mixtures. Progress report (February 1990-February 1991). J. F. Ely. Nov 90, 24p DOE/ER/13992-T1 Contract AI05-89ER13992

Sponsored by Department of Energy, Washington, DC.

Keywords: \*Suspensions, Colloids, Computerized Simulation, \*Fluids, Microstructure, Mixtures, Neutrons, Polystyrene, Progress Report, Scattering, Shear, Silica, Thermal Conductivity, EDB/640410, EDB/360603, \*Thermophysical properties.

In this report we highlight the progress made during the period February 1990 through February 1991. The

objective of this research is twofold: 1. Development of predictive and correlative procedures for the thermo-physical properties of complex fluids and fluid mixtures; and 2. Furthering our basic understanding of fluid behavior with advances in microscopic theory, computer simulation and selected experimentation. Substantial progress has been made in both of these areas. 39 refs., 4 figs.

101,385

PB91-134585 Not available NTIS National Inst. of Standards and Technology (NEL), Boulder, CO. Thermophysics Div.

Phase Equilibria from the One-Fluid Model.

Final rept.

K. D. Romig, and H. J. M. Hanley. 1989, 3p Sponsored by Department of Energy, Washington, DC. Pub. in Cryogenics 29, n1 p65-67 Jan 89.

Keywords: Mathematical models, Predictions, Reprints, \*Binary fluids, Binary mixtures, Phase equilibrium, Lennard-Jones potential.

The prediction of possible phase behavior in binary fluid mixtures is discussed in the context of the Scott and van Konynenberg scheme. It is shown that the corresponding states one-fluid model for Lennard-Jones mixtures gives qualitative agreement with experiment.

101,386

PB91-147892 Not available NTIS National Bureau of Standards (NEL), Gaithersburg,

MD. Fire Measurement and Research Div.

Development of a Line Camera for Real-Time

Measurements of Concentration in Turbulent Flow Fields.

Final rept.

W. M. Pitts. 1987, 9p Contract AFOSR-ISSA86-0008

Sponsored by Air Force Office of Scientific Research, Bolling AFB, Washington, DC. Pub. in Proceedings of International Congress on Apli-

cations of Lasers and Electrooptics (5th), Arlington, VA., November 10-13, 1986, p7-15 1987.

Keywords: \*Flow visualization, \*Turbulent flow, \*Cameras, Rayleigh scattering, Light scattering, Real time operations, Concentration(Composition), Image intensifiers, Laser applications, Gas flow, Propane, Re-

The development of an intensified digital line camera for laser-induced Rayleigh light scattering measurements of real-time concentration fluctuations in turbulent flow fields is described. Particular attention is given to the need for and choice of an image intensifigiven to the freed for and choice of an image intensin-er. Preliminary results for a turbulent jet of propane flowing into air are presented.

101,387

PB91-148031 Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Chemical Engineering Science Div. Effect of Pipe Surface Finish on Gas Flow Measurement with an Orifice Meter.

C. F. Sindt, J. A. Brennan, S. E. McFaddin, and K. M. Kothari. 1990, 8p Sponsored by Gas Research Inst., Chicago, IL.

Pub. in Proceedings of International Gas Research Conference, Tokyo, Japan, November 6-9, 1989, p1-8

Keywords: \*Flow measurement, \*Orifice meters, \*Pipes(Tubes), Surface properties, Roughness, Gas flow, Reynolds number, Reprints.

The National Institute of Standards and Technology (NIST) under the sponsorship of the Gas Research Institute (GRI) has completed an investigation of the change in the orifice discharge coefficient caused by the surface finish in the pipe upstream of the orifice plate. Three sizes of pipes of three roughnesses were tested. The results from this investigation show that the orifice discharge coefficient is affected by pipe sur-face finish and the effect depends upon the Reynolds number and the orifice beta ratio

101.388

PR91-162263 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Thermophysics Div.

### **PHYSICS**

### Fluid Mechanics

Computer Simulation of Fluid-Fluid Phase Coexistence in Mixtures of Nonadditive Soft Disks. Final rept.

R. D. Mountain, and A. H. Harvey. 1991, 6p Pub. in Jnl. of Chemical Physics 94, n3 p2238-2243, 1 Feb 91.

Keywords: \*Equilibrium, \*Binary mixtures, \*Liquids, Gibbs equations, Thermodynamic properties, Monte Carlo method, Simulation, Stochastic processes, Molecular flow, Mixing, Mixtures, Reprints.

Fluid-fluid phase equilibrium in binary mixtures of positively nonadditive soft disks is studied using both mo-lecular dynamics and Gibbs ensemble Monte Carlo simulations. The molecular dynamics simulations are unable to provide quantitative results for the phase transition, but they do indicate that some sort of ordering takes place as the temperature is lowered. In contrast, the Gibbs ensemble simulations demonstrate un-ambiguously the presence of a first-order transition and give quantitative results for the coexistence curve; however, convergence is very slow for mixtures that are not symmetric. Comparison with the Gibbs ensemble results indicates that a simple first-order perturbation theory provides good results far from the consolute point. Closer to the consolute point, the theory does not reproduce the flatness of the coexistence curve; the limitation is intrinsic in any mean-field theory. Comments are made regarding the relative merits of molecular dynamics and Gibbs ensemble simulations for studying fluid-fluid phase coexistence.

PB91-162347 Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Chemical Engineering Science Div. Effect of Pipe Surface Finish on the Orifice Discharge Coefficient. Final rept.

C. F. Sindt, J. A. Brennan, S. E. McFaddin, and R.

Wilson. 1989, 8p Sponsored by Gas Research Inst., Chicago, IL. Pub. in VDI Berichte 768, p49-56 1989.

Keywords: \*Pipe flow, \*Surface roughness, \*Orifice meters, \*Orifice flow, Finishes, Surface properties, Pipes(Tubes), Orifices, Flow measurement, Reynold number, Gas flow, Reprints.

The U.S. National Institute of Standards and Technololnstitute (GRI), investigated the change in the orifice discharge coefficient caused by the interior surface finish in the pipe upstream of the orifice plate. Three sizes of meters and three surface finishes were tested over a range of pipe Reynolds numbers from  $4.3 \times 10$  (to the power of 5) to  $1.2 \times 10$  (to the power of 7). The results of the investigation show that the orifice discharge coefficient changed more than one percent at a Reynolds number of 7 x 10 (to the power of 6) between a smooth pipe, 2.8 micrometer Ra, and a rough pipe, 8.9 micrometer Ra, for a beta ratio of 0.74. For beta ratios less than 0.5 the change in the orifice discharge coefficient was not measurable for the same change in pipe roughness.

101,390 PB91-195263 Not available NTIS National Inst. of Standards and Technology (NEL), Boulder, CO. Scientific Computing Div.
Use of Computer Algebra to Locate Critical Loci in

Fluid Mixtures. Final rept.

G. C. Nielson, M. O. McLinden, and G. Morrison. 1990, 10p

Pub. in Jnl. of Symbolic Computation 10, n5 p499-508

Keywords: \*Fluids, \*Mixtures, \*Loci, \*Computer calculations, Algebra, Rational functions, Linear algebraic equations, Symbolic codes, Phase diagrams, Refrigerants, Reprints.

The authors have explored the use of the symbolic manipulator MACSYMA to generate FORTRAN code for finding critical loci in 2-component fluid mixtures. For a given equation of state and mixing rules, MAC-SYMA can generate the equations satisfied at a critical point. MACSYMA also produces FORTRAN code that can be used to develop codes for finding critical loci. The results for test cases where traditional methods have been applied are identical to earlier work. They describe the application of the technique to the Carnahan-Starling-De Santix equation, a non-cubic function consisting of a hard-sphere kernal and a RedlichKwong-like attractive term. Examples of its application to refrigerant mixtures are described.

101.391

PB91-195636 Not available NTIS National Inst. of Standards and Technology, Boulder, CO. Thermodynamics Div.

Non-Equilibrium Molecular Dynamics Simulations of Structured Molecules. Part 1. Isomeric Effects on the Viscosity of Butanes.

Final rept. R. L. Rowley, and J. F. Ely. 1991, 16p Pub. in Molecular Physics 72, n4 p831-846 1991.

Keywords: \*Viscosity, \*Butane, \*Iennard-Jones potential, \*Nonequilibrium flow, Rheology, Simulation, Reprints, Molecular dynamics.

Corresponding-states theories fail to predict the large difference observed between n-butane and isobutane viscosities at similar reduced conditions. To investigate the molecular cause of the structural effects upon viscosity, non-equilibrium molecular dynamics simulations of Lennard-Jones site-site models representing

n-butane and isobutane are performed over much of the density range for which experimental data are available. Simulated viscosities at zero shear agree very well with experimental data over the entire density range. Site size, non-equilibrium molecular alignment and molecular geometry are the primary factors causing both the similarities and differences between the isomers' viscosity and rheology.

101,392

PB91-200832 Not available NTIS National Bureau of Standards (NEL), Boulder, CO. Thermophysics Div.

Taking the Measure of Fluid Properties Data Bases. Final rept.

M. E. Baltatu, H. J. M. Hanley, and N. A. Olien, 1987,

Pub. in Mechanical Engineering, p64 Dec 87.

Keywords: \*Fluids, \*Thermophysical properties, \*Data bases, Critical point, Melting points, Thermochemical properties, Thermodynamic properties, Pressure, Temperature, Reprints

The status of thermophysical properties data bases today is discussed with comments on needs for the future. Recommendations for obtaining the best possible bases are discussed. Future work will require close cooperation between the scientist and the engineer. Examples of such cooperation are given.

PB91-203000 Not available NTIS National Inst. of Standards and Technology (NML), PB91-203000 Boulder, CO. Thermophysics Div.

Analysis of Laminar Vortex Shedding Behind a Cir-

cular Cylinder by Computer-Aided Flow Visualiza-

B. E. Eaton. 1987, 29p Sponsored by National Research Council of Canada, Ottawa (Ontario)

Pub. in Jnl. of Fluid Mechanics 180, p117-145 1987.

Keywords: \*Flow visualization, \*Computational fluid dynamics, \*Vortex shedding, \*Cylinders, Finite element method, Numerical analysis, Navier-Stokes equations, Reynolds number, Two dimensional flow, Wakes, Critical point, Vortex flow, Vortices, Reprints.

Streamline, streakline, and material-line flow-visualization techniques have been numerically simulated in the vortex-shedding flow field from a finité-element simulation of the two-dimensional Navier-Stokes equations at a Reynolds number of 110. The results have been used (i) to characterize the wake in terms of its criticalpoint trajectories, and (ii) to verify that the two-dimensional Navier-Stokes model predicts the mechanism of vortex shedding experimentally observed by Gerrard (1978). A technique for determining vorticity balances in the flow field is also presented.

101.394

PB91-204123 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Thermophysics Div. Thermodynamic Behavior of Fluids in the Supercritical Region.

Final rept. S. Tang, and J. V. Sengers. 1991, 4p Contract DE-FG05-88ER13902

Sponsored by Department of Energy, Washington, DC. Pub. in Proceedings of International Symposium on Supercritical Fluids (2nd), Boston, MA., May 20-22, 1991, p254-257.

Keywords: \*Thermodynamic properties, \*Fluids, \*Supercritical state, Free energy, Temperature, Critical temperature, Critical point, Thermodynamics, Pressure, Equations of state, Reprints.

A procedure for constructing a thermodynamic free energy of fluids is discussed which incorporates a crossover from singular thermodynamic behavior at the critical point to regular thermodynamic behavior far away from the critical point. The procedure is based on an approximate solution of the renormalization-group theory of critical phenomena and yields an accurate representation of the thermodynamic properties of fluids in a large range of temperatures and densities around the critical point.

101.395

PB91-222679 PC A03/MF A01 National Inst. of Standards and Technology (CSTL), Boulder, CO. Chemical Engineering Div. Unsteady Laminar Flow in a Circular Tube: A Test

of the HERCOL (Hermitian Collocation) Computer Code.

J. F. Welch, J. A. Hurley, M. P. Glover, R. D. Nassimbene, and M. R. Yetzbacher. May 91, 27p NISTIR-3963

Keywords: \*Laminar flow, \*Computational fluid dynamics, \*Pipe flow, \*Velocity distribution, Fluid flow, Pressure gradients, Unsteady flow, Computer programs, Partial differential equations, Numerical analysis Tubes (IEEE/Computer States) sis, Tubes, HERCOL computer program.

HERCOL, a computer code for the integration of second-order differential equations in one space dimension by Hermitian collocation was used to calculate the unsteady velocity profiles for laminar flow in a circular tube. The code was tested for stability and accuracy on the problem for which an analytical solution exists prior to application to a like problem in which the initial and boundary conditions preclude the existence of analytical solutions. The test problem is one in which a pressure gradient is imposed on a fluid initially at rest in a circular tube; the fluid accelerates and at at rest in a circular tube, the fluid accelerates and at steady state has a parabolic velocity profile. A second example was constructed from the first; a pressure gradient equal but opposite in sign is imposed on the fluid with a fully developed parabolic velocity profile. At steady state, the velocity is again parabolic but in the opposite direction to that at the initial conditions. Excellent agreement with the analytical solution was obtained in the first problem; in the second, the behavior was as expected. This example is suitable for first-time users of the code.

101.396

PB92-112291 PC A03/MF A01 National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Applied and Computational Mathe-

Effect of Gravity Modulation on Thermosolutal Convection in an Infinite Layer of Fluid.

B. V. Saunders, B. T. Murray, G. B. McFadden, S. R. Coriell, and A. A. Wheeler. Oct 91, 42p NISTIR-4679 See also PB90-265281.

Keywords: \*Convection, Binary alloys, Reduced gravity, Instability, \*Thermosolutal convection, Thermohaline convection, Buoyant convection, Gravity modulation Direction local differences. tion. Directional solidification.

The effect of time-periodic vertical gravity modulation on the onset of thermosolutal convection in an infinite horizontal layer with stress-free boundaries is investi-gated using Floquet theory for the linear stability analy-sis. The authors consider situations for which the fluid layer is stably stratified in either the fingering or diffusive regimes of double-diffusive convection. Results are presented both with and without steady background acceleration. Modulation may stabilize an un-stable base solution or destabilize a stable base solu-tion. In addition to synchronous and subharmonic response to the modulation frequency, instability in the double-diffusive system can occur via a complex conjugate mode. In the diffusive regime, where oscillatory

onset occurs in the unmodulated system, regions of resonant instability occur and exhibit strong coupling with the unmodulated oscillatory frequency.

101,397 PB92-116490 Not available NTIS National Inst. of Standards and Technology (CSTL), Boulder, CO. Chemical Engineering Div.
Choosing Flow Conditioners and Their Location for Orifice Flow Measurement. Final rept. J. A. Brennan, C. F. Sindt, M. A. Lewis, and J. L. Scott. 1991, 5p Contract GRI-5088-271-1680

Sponsored by Gas Research Inst., Chicago, IL. Pub. in Flow Meas. Instrum. 2, p40-44 Jan 91.

Keywords: \*Orifice meters, \*Orifice flow, \*Rod bundles, Fluid flow, Flowmeters, Orifices, Flow measurement, Flow control, Turbulence, Reprints, \*Flow condi-

Three different tube bundles, a zanker, and an etoile flow conditioner have been tested in a 100 mm orifice flowmeter. The tube bundles included a seven- and a 19-tube configuration. Tests were designed to determine a location for the flow conditioner that would remove the effects of flow disturbances and keep the length of the meter tube as short as possible. The disturbances included an inlet tee, two out-of-plane elbows, and a single elbow. All disturbances were preceded by another long radius elbow located 12 pipe diameters upstream. Results indicate that it may be possible to move the conditioner closer to the disturbance than current standards permit.

# **Optics & Lasers**

101,398 AD-A207 806/1 PC A06/MF A01 National Inst. of Standards and Technology, Gaithers-

Annual Report to the Strategic Defense Initiative Organization on the Free-Electron Laser Driven by the NIST CW Microtron.

Annual rept. 1 Apr 88-31 Mar 89. R. G. Johnson. 5 May 86, 101p Contract N00014-87-F-0066

Keywords: Acceleration, Damage, Electric current, Engineering, \*Free electron lasers, Mirrors, Peak power, Short pulses, Test and evaluation, \*Antimissile defense systems, \*Strategic Defense Initiative.

Excellent progress has been made during the past year on all areas critical to the NIST-NRL FEL project. A contract for the construction of a wiggler was signed early in this reporting period. The contractor has completed the engineering design of the wiggler and is well along in construction. Several methods to increase the peak current in the RTM were studied. The conceptual design of the injector for the method selected was completed. A study on the problem of mirror damage has been completed, and commercial suppliers of mir-rors that can withstand the high intracavity power of the FEL have been identified. The design of the room in which the FEL is located has been improved, and the design of the users area has been completed. Cal-culations of FEL performance have been extended to include short-pulse effects and the effects of wiggler magnetic field errors. A major activity in this period has been preparation of the RTM for one-pass acceleration to 17 MeV. One-pass tests were started, and preliminary measurements of beam quality were better than design goals by a factor of two.

101,399 AD-A227 310/0 PC A03/MF A01 National Inst. of Standards and Technology, Gaithersburg, MD.
NIST-NRL Free-Electron Laser.

Status rept.
P. H. Debenham, R. L. Ayres, W. A. Cassatt, B. C. Johnson, and R. G. Johnson, 1990, 12p Contract N00014-87-F-0066

Keywords: Accuracy, Cavities, Electron beams, Errors, Facilities, \*Free electron lasers, Frequency, Length, Losses, Mirrors, Models, Oscillators, Pulses, Simulation, Three dimensional, User needs, White light, Racetrack microtrons, Picosecond pulses, Tunable

A free-electron laser (FEL) user facility is being con-A free-electron laser (FEL) user lacinity is being constructed. The FEL, which will be operated as an oscillator, will be driven by the 17 MeV to 185 MeV to 185 MeV electron beam of the NIST continuous-wave racetrack microtron. Anticipated performance of the FEL includes: wavelength tuneable from 200 nm to 10 micrometers; a continuous train of 3-ps pulses at either 16.5 or 66.1 MHz; and average power of 10 W to 200 W. Construction of the RTM will be completed in Janu-W. Construction of the HTM will be completed in January 1991. The measured rms field error is 0.6%, which is sufficiently small for good gain. With a full-scale model of the 9-m-long optical cavity, we have developed a method of aligning the cavity end mirrors to the required accuracy using white light and an autocollimator/telescope. We have performed three-dimensional simulations of performance including the effects of the electron beam (emittance, pulse length and shape, and timing jitter), undulator field errors, and cavity losses. These calculations predict adequate gain for lasing across the full wavelength range. (RH)

101,400 AD-A236 746/4 PC A02/MF A01 National Inst. of Standards and Technology, Gaithersburg, MD.
Critical Assessment of Optical Properties of CVD

Diamond Films. Interim rept.

A. Feldman, and L. H. Robins. 12 Apr 91, 10p. Contract N00014-90-F-0011

Keywords: Blue(Color), Coatings, Deposits, Diamonds, Energy bands, Infrared windows, Laser materials, Luminescence, Optical materials, Optical properties, Phonons, Quality, Quantum efficiency, Surface roughness, Vapor deposition, X rays, Thin films, \*Diamond films, Chemical vapor deposition, Progress report.

The basic phenomena that determine the optical properties of diamond, which include the electronic band structure, the phonon structure, and defects, are discussed. Experiments on chemical vapor deposited diamond relevant to its applications as an optical material are reviewed. The most immediate application is the diamond x-ray window. Other applications, such as infrared transmissive elements and coatings, will require considerable improvement in material quality. Surface roughness is a major impediment. The ability to deposit smooth surfaces would make diamond considerably more attractive as optical material. Diamond also has promise as a blue luminescent or laser material. Identifying and controlling the relevant luminescent centers will be needed to improve the quantum efficiencies of such devices.

101,401 AD-A243 097/3 PC A03/MF A01 National Inst. of Standards and Technology, Gaithersburg, MD.
Use of Diamond as an Optical Material.

Technical rept.
A. Feldman. 27 Sep 91, 17p
Contract N00014-90-F-0011

Keywords: Absorption, Adhesion, Carbon, Chemical reactions, Coatings, Films, Impurities, Lithography, Materials, Methodology, \*Optical materials, \*Optical properties, Optics, Phase, Polishing, Scattering, Single crystals, Substrates, Surface roughness, Vapor deposition, X rays, \*Diamonds, Chemical vapor deposition.

Chemical vapor deposition (CVD) processes promise inexpensive diamond optics and coatings with large dimensions. Near term optical applications include x-ray windows, membranes for x ray lithography, and infra-red windows and domes. CVD diamond, which is mainly polycrystalline, shows materials problems that include scattering due to large surface roughness, absorption due to defects, non diamond carbon phases, and impurities, and poor diamond/substrate adhesion. Free carrier absorption in CVD diamond has also been reported. While diamond films less than 3 um thick can be made transmissive in the visible and in the ultraviolet, at these wavelengths, thicker components scatter excessively and show absorption due to defects. Continuing research is improving the optical quality of CVD diamond. New polishing methods have yielded smooth surfaces in reasonable polishing times. Recent research holds promise for large optics made from single crystal diamond.

# 101,402 PB90-244708

(Order as PB90-244658) Technische Univ. Muenchen (Germany, F.R.). Lehrstuhl fuer Thermodynamik.

Refractive Index of Water and Steam as Function of Wavelength, Temperature and Density. Quarterly rept.

Quarterly rept.
P. Schiebener, J. Straub, J. M. H. Levelt Sengers, and J. S. Gallagher. c1990, 41p
Prepared in cooperation with National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Thermontheries Pitt. morphysics Div.

Included in Jnl. of Physical and Chemical Reference Data, v19 n3 p677-717 1990. Available from American Chemical Society, 1155 16th St., NW, Washington, DC

Keywords: \*Water, \*Water vapor, \*Steam, Near infra-red radiation, Near ultraviolet radiation, Tables(Data), \*Refractive index, Visible radiation, Temperature de-

Based on a comprehensive collection of data previously obtained by Thormahlen et al. on the experimental refractive index of water and steam from the 1870s to the present, a new formulation is presented for the range of 0.2 to 2.5 micrometers in wavelength, -10 to +500 deg C in temperature and 0 to 1045 kg/cu m in density. The Lorentz-Lorenz function or molar refraction, a strong function of wavelength but only weakly dependent on density and temperature, is fitted to a selected set of accurate refractive index data. The NBS/NRC equation of state for water and steam, the new international standard is used to convert the experimental pressures to density. The deviations of all experimental data from the formulation are shown. A detailed assessment of the accuracy of the formula-tion is presented. It is demonstrated that several recent formulations of optical properties of liquid water over large ranges of wavelength need improvement in the range covered here. The new formulation is used to generate tables of the refractive index of water and steam at six wavelengths in the visible, near-infrared and near-ultraviolet, from 0 to 500 deg C and up to 100 MPa in pressure.

101.403

PB91-132308 PC A10/MF A02
National Inst. of Standards and Technology (NEL),
Boulder, CO. Electromagnetic Technology Div.
Technical Digest-Symposium on Optical Fiber
Massurements 1000 Measurements, 1990. G. W. Day, and D. L. Franzen. Sep 90, 211p NIST/

SP-792

Also available from Supt. of Docs. See also PB89-129555. Prepared in cooperation with Optical Society of America, Washington, DC.

Keywords: \*Fiber optics, \*Optical measurement, \*Meetings, Optical communication, Electrooptics, Reflectometers, \*Optical fibers, Fiber optics transmission lines, Sensors,

The digest contains summaries of 45 papers presented at the Symposium on Optical Fiber Measurements, held September 11-12, 1990, at the National Institute of Standards and Technology, Boulder, Colorado.

101,404

PB91-134106 Not available NTIS
National Bureau of Standards (NML), Boulder, CO.
Time and Frequency Div.
Modulatable Narrow-Linewidth Semiconductor

Lasers.

Final rept. L. Hollberg, and M. Ohtsu. 1988, 3p See also PB88-239470. Pub. in Applied Physics Letters 53, n11 p944-946 Sep

Keywords: \*Semiconductor lasers, Frequency control, Frequency stability, Line width, Optical communication, Reprints, Frequency division multiplexing, Line narrowing.

The authors found that using the technique of optical feedback locking, to narrow semiconductor linewidths, does not sacrifice the ability to modulate the laser's frequency via the injection current. The frequency of a laser is stabilized to a separate Fabry-Perot reference cavity using resonant optical feedback and can be modulated efficiently at frequencies related by rational fractions to the free-spectral range of the reference cavity. This system can provide an array of narrow-linewidth, frequency-stable laser lines and shows promise for applications in frequency-division-multiplexed coherent communications, as well as laser frequency control and precision measurement systems.

### Optics & Lasers

101,405 PB91-134130 Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Time and Frequency Div.
Accurate Frequency of the 119 mu m Methanol
Laser from Tunable Far-Infrared Absorption Spec-

Final rept.

M. Inguscio, L. R. Zink, K. M. Evenson, and D. A. Jennings. 1990, 5p Pub. in IEEE (Institute of Electrical and Electronics En-

gineers) Jnl. of Quantum Electronics 26, n3 p575-579 Mar 90.

Keywords: \*Frequency measurement, Far infrared radiation, Absortion spectra, Infrared lasers, Reprints, \*Methanol lasers, \*Laser frequencies.

The authors report on high accuracy absorption spectroscopy of CH3OH in the far infrared. In addition to 22 transitions in the ground state, the authors have measured the frequency of the (n, tau, J, K), (0, 1, 16, 8) -> (0, 2, 15, 7) transition in the nu sub 5 excited vibrational level, which is responsible for the laser emission at 119 micrometers. An accurate remeasurement of the laser emission frequency has also been performed, and the results are in good agreement.

101.406 PB91-147207 Not available NTIS
National Inst. of Standards and Technology (NEL),
Boulder, CO. Electromagnetic Technology Div.
Standard Reference Fibers for Calibration of the Optical Time Domain Reflectometer. Final rept.

B. L. Danielson, C. D. Whittenberg, and T. Drapela.

1989, 4p Pub. in Proceedings of International Instrumentation Symposium (35th), Orlando, FL., May 1-4, 1989, p895-

Keywords: \*Reflectometers, \*Calibration, Optical fibers, Reprints, \*Standard reference fibers, \*Reference materials, \*Optical time domain reflectometers, OTDR(Optical time domain reflectometers).

Calibration of optical time domain reflectometers by military and industrial users can be achieved by a number of published test procedures. For some performance parameters, a particularly convenient way for establishing measurement verification and traceability to national standards is through the use of a standard reference fiber. At NIST the authors have begun a program to evaluate such test lightguides. Prototype standard reference fibers have been characterized for spectral attenuation, group delay, group index, and length. The authors describe measurement methods and tolerances for these devices.

101,407 PB91-147868 Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Chemical Engineering Science Div. Fiber-Optic Fluorescence Array to Study Free Convection in Porous Media. Final rept.

R. A. Perkins, and M. C. Jones. 1989, 6p Sponsored by Department of Energy, Washington, DC. Office of Basic Energy Sciences.
Pub. in Review of Scientific Instruments 60, n11

p3492-3497 Nov 89.

Keywords: \*Convection, \*Fiber optics, \*Fluorescence, Fluorescent dyes, Labelled substances, Porous materials, Design, Fluid mechanics, Reprints.

A 64-point fiber-optic fluorescence array is integrated into a heated-packed bed to study free convection in porous media. The array consists of 64 individual fluorescence coupler-detector modules. The array mod-ules are designed for rhodamine 6G dye and allow real-time measurement of tracer concentrations to about 40 ppb. The coupler-detectors are inexpensive and allow a single fiber to carry both the excitation light and the emitted fluorescence light between the detectors and the remote probe terminations at known locations within the bed. Dilute pulses of tracer dye are injected into the packed bed and the dye concentration at each of the 64 fiber-optic probe terminations is monitored as a function of elapsed time. The tracer concentration as a function of time and position allows the fluid movement to be followed within the porous

101,408 PB91-148007

Not available NTIS

National Inst. of Standards and Technology (NEL), Boulder, CO. Electromagnetic Technology Div. Subpicosecond Pulse Compression and Raman Generation Using a Mode-Locked Erbium-Doped Fiber Laser-Amplifier.

Final rept.

J. B. Schlager, P. D. Hale, and D. L. Franzen. 1990,

Pub. in IEEE (Institute of Electrical and Electronics Engineers) Photonics Technology Letters 2, n8 p562-564 Aug 90.

Keywords: \*Pulse compression, Near infrared radi-ation, Mode locked lasers, Picosecond pulses, Doped materials, Raman effect, Raman lasers, Solitons, Reprints, Femtosecond pulses, Erbium fibers.

Pulses of 20 ps duration from a 1536 nm erbium-doped fiber laser mode-locked at 10 MHz are soliton-com-pressed in a 1 km fiber to 1.5 ps. The pulses are then amplified in an erbium-doped fiber amplifier and com-pressed in a second fiber to less than 300 fs. Pulses give rise to stimulated Raman scattering in fibers; the direct output from the erbium fiber laser-amplifier has sufficient peak power to pump fiber Raman lasers.

101,409 PB91-148478 PC A99/MF A04 National Inst. of Standards and Technology, Boulder,

Laser Induced Damage in Optical Materials: 1989. Special pub.

H. E. Bennett, L. L. Chase, A. H. Guenther, B. E. Newnam, and M. J. Soileau. Oct 90, 674p NIST/SP-

Also available from Supt. of Docs. as SN003-003-03061-9. See also report for 1988, PB90-185570. Errata sheet inserted. Proceedings of Annual Symposium on Optical Materials for High-Power Lasers (21st), Boulder, CO., Nov. 1-3, 1989. Prepared in coop. with American Society for Testing and Materials, Philadelphia, PA., SPIE-The International Society for Optical Engineering, Bellingham, WA.

Keywords: \*Optical materials, \*Radiation damage, \*Laser damage, \*Meetings, Physical radiation effects, Laser materials, Thin films, Optical coatings, Surfaces,

The Twenty-First Annual Symposium on Optical Materials for High-Power Lasers was divided into sessions concerning Materials and Measurements, Mirrors and Surfaces, Thin Films, and, finally, Fundamental Mech-anisms. As in previous years, the emphasis of the papers presented at the Symposium was directed toward new frontiers and new developments. Particular emphasis was given to materials for high power apparatus. The wavelength range of the prime interest was from 10.6 micrometers to the uv region. Highlights included surface characterization, thin film substrate boundaries, and advances in fundamental laser-matter threshold interactions and mechanisms. The scalling of damage thresholds with pulse duration, focal area, and wavelength was discussed in detail.

PB91-148908 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Radiometric Physics Div. Use of Heterodyne Detection to Measure Optical Transmittance over a Wide Range.

Final rept. A. L. Migdall, B. Roop, Y. C. Zheng, J. E. Hardis, and . J. Xia. 1990, 9p

Pub. in Applied Optics 29, n34 p5136-5144, 1 Dec 90.

Keywords: \*Transmittance, Optical filters, Zehnder interferometers, Demodulation, Heterodyning, Acoustooptics, Optical measurement, Reprints, Densitometry.

The authors are developing a heterodyne detection technique to measure optical transmittance with high accuracy over an unprecedented dynamic range. They have measured filters spanning a wide range of trans-mittances (12 orders of magnitude) and have evaluated the absolute uncertainties and discuss the ultimate accuracies that may be achieved. Their setup uses a two-beam Mach-Zehnder interferometer with acoustooptic frequency shifting to produce a frequency dif-ference between the two light beams. The authors de-termine the optical transmittance of a filter by inserting it into one of the interferometer arms and measuring the change in amplitude of the signal at the difference frequency on the interferometer output beam. The method allows direct comparisons between optical

and rf attenuators, ultimately tying optical transmittance measurements to rf attenuation standards in an absolute way.

101.411

PB91-149138 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Temperature and Pressure Div.

Dispersion of the Electronic Contribution to the

Third-Order Nonlinear Susceptibility of H2. Final rept.

G. J. Rosasco, and W. S. Hurst. 1986, 6p Pub. in Jnl. of the Optical Society of America B 3, n10 p1251-1256 Oct 86.

Keywords: \*Hydrogen, Raman spectra, Kerr effect, Reprints, Nonlinear susceptibility, Second harmonic generation, Third harmonic generation.

A new value is reported for the electronic contribution the electronic hyperpolarizability) to the third-order nonlinear susceptibility of H2. The result is derived from a measurement of the ac (optical)-Kerr constant referenced to the resonant Q-branch susceptibility of D2. A long-known dispersion formula is applied to compare the authors' value of the electronic hyperpolarizability with values determined by other nonlinear optical techniques. The dispersion formula is shown to account systematically for the results of other nonlinear techniques.

101.412

PB91-149195 Not available NTIS National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div. Laser Measurements.

Final rept.

A. A. Sanders. 1983, 3p Pub. in Proceedings of Measurement Science Confer-ence, Palo Alto, CA., January 20-21, 1986 p198-200 1983.

Keywords: \*Laser radiation, \*Lasers, Power measurement, Beam profiles, Calorimeters, Metrology, US NBS, Reprints.

The report will review some of the national standards and measurement services for lasers available at NBS, highlight some of the current research, and indicate some of the future needs and direction of NBS laser metrology research.

PB91-158709 Not available NTIS National Bureau of Standards (IMSE), Gaithersburg, MD. Ceramics Div.

Stoichiometry of Reactively Evaporated Films. Final rept.

A. Feldman, E. N. Farabaugh, and Y. N. Sun. 1988,

Pub. in Proceedings of Optical Interference Coatings Topical Meeting, Tucson, AZ., April 12-15, 1988, p14-

Keywords: \*Optical films, \*Silicon oxides, \*OXidation, Photoelectron spectroscopy, Dielectric films, Thin films, Stoichiometry, Reprints.

If an optical film is not fully oxidized, its refractive index will be different from expected, and significant optical absorption may result. In order to ensure full oxidation of oxide films, evaporations are frequently carried out in reactive atmospheres containing significant partial pressures of oxygen. SiO(x) films provide a convenient system for studying the oxidation state of reactively evaporated films, not only because they are important coating materials, but because structural models have been developed for the system. In the paper, the degree of oxidation of SiO(x) films, prepared by reactive electron-beam evaporation of Si under different partial pressures of oxygen, has been examined by X-ray photoelectron spectroscopy (XPS). The analysis suggests that he silicon in the films is not as fully oxidined as might be oxygeted by the beginning of the present of the dized as might be expected on the basis of the measured oxygen content.

101.414

PB91-158972 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Applied and Computational Mathe-

# **Optics & Lasers**

Algorithm and Computer Program for the Calculation of Envelope Curves.

Final rept. M. McClain, A. Feldman, D. Kahaner, and X. T. Ying. 1991, 4p

See also PB90-155409. Pub. in Computers in Physics, p45-48 Jan/Feb 91.

Keywords: \*Curve fitting, \*Light transmission, Refractive index, Absorptivity, Transmittance, Oscillations, Interpolation, Algorithms, Reprints, Envelope curves.

A procedure has been developed to calculate numerically the envelope functions of an oscillatory curve. The method has been shown to be applicable to optical transmission data, but it is general enough to be used for many other data sets. The program is available on request.

101,415 PB91-174854 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Atomic and Plasma Radiation Div.

Laser-Driven Ionization and Photoabsorption Spectroscopy of Atomic Ions.

W. T. Hill, and C. L. Cromer. 1987, 12p Pub. in Springer Ser. Opt. Sci. 54, p183-194 1987.

Keywords: \*Atomic ions, \*Photoabsorption, Barium ions, Cesium ions, Xenon ions, Isoelectronic sequence, Laser radiation, Ionization, R matrix, Reprints.

The application of laser-driven ionization techniques to photoabsorption spectroscopy of atomic ions will be discussed. A summary of the experimental results which confirm that a collisional mechanism is responsible for the nearly complete ionization following laser irradiation is given, along with a bibliography of the photoabsorption measurements reported to date. The importance of these investigations, demonstrated in two studies involving the Ba nuclear sequence (i.e. Ba, Ba(1+), and Ba(2+)) and the Xe isoelectronic sequence (i.e. Xe, Cs(1+) and Ba(2+)), will be discussed. Finally, a tabulation of quantum defect parameters for Xe, Cs(1+), and Ba(2+) based on a re-analysis of the Xe-sequence spectra via a shifted R-matrix quantum defect approach will be presented.

PB91-175141 Not available NTIS
National Inst. of Standards and Technology (NEL),
Boulder, CO. Electromagnetic Technology Div.
Semiconductor Claddings on Glass Waveguides for Polarizers and Detectors. Final rept.

D. L. Veasey, D. R. Larson, R. J. Phelan, and T. E. Batchman, 1990, 1p

Pub. in Proceedings of Optical Society of America Annual Meeting Technical Digest, Boston, MA., November 4-9, 1990, pMA5.

Keywords: \*Polarizers, Amorphous silicon, Waveguides, Detectors, Semiconductors, Reprints, Claddings.

TE and TM polarizers and polarization sensitive detectors were fabricated by cladding glass channel wave-guides with hydrogenated amorphous silicon. Extinc-tion ratios as high as 48 dB have been observed for the TE pass device and up to 34 dB for the TM pass device

101,417 PB91-175596 Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Quantum Physics Div.

Correlated Spontaneous Emission in a Zeeman

Laser.

M. P. Winters, and J. L. Hall. 1990, 4p Contract N00014-89-J-1227, Grant NSF-PHY86-

Sponsored by Office of Naval Research, Arlington, VA., and National Science Foundation, Washington, DC.

Pub. in Physical Review Letters 65, n25 p3116-3119, 17 Dec 90.

Keywords: \*Helium neon lasers, Spontaneous emission, Laser interferometry, Sensitivity, Reprints, \*Zeeman lasers.

The authors have observed phase-diffusion noise 40% below the Schawlow-Townce limit in the relative phase of a two-mode HeNe Zeeman laser due to the correlated-emission-laser effect.

101.418 PB91-187096 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Radiometric Physics Div. Temperature Dependence of High Accuracy-Photometer Heads. Final rept. G. Andor. 1989, 2p

Pub. in Applied Optics 28, n22 p4733-4734, 15 Nov 89. Keywords: \*Photometers, \*Photodiodes, Silicon diodes, Temperature dependence, Transmittance, Re-

The redefinition of the Candela in 1979 permits the use of upsilon(lambda) response photodetectors as primary photometric standards. Their long-term stability and temperature dependence is of prime importance in this application. Modern high-accuracy photometer heads consist of a silicon photodiode, a upsilon(lambda) matched glass filter and a current to voltage converter. The purpose of the letter is to report an investigation of the temperature characteristics for three types of high-quality silicon photodiodes and their matching filters. The temperature dependence of a properly designed current to voltage converter in the practical illuminance range of 0.0001 to 10,000 lux is

101.419 PB91-187419 Not available NTIS National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Ceramics Div.

Design Diagrams for Heavy Metal Fluoride Glass

negligible.

D. Cranmer, T. Chuang, S. Freiman, and A. Raynes. 1990, 17p

Sponsored by Naval Research Lab., Washington, DC., and Center for Naval Analyses, Alexandria, VA. Naval Warfare Operations Div.

Pub. in Proceedings of High Power Laser Optical Components Topical Meeting, China Lake, CA., October 30-31, 1989, p98-114 1990.

Keywords: \*Design criteria, \*Glass, \*Window glass, \*Fluorides, \*Optical materials, Lasers, Service life, Finite difference theory, Fatigue limit, Weibull density functions, Reliability, Stress analysis, Mathematical models, Reprints, Heavy metals.

In order to design structures with materials such as heavy metal fluoride glasses, it is necessary that the stresses under which the structure will operate and the probability that the structure will survive these stresses be known. An experimental and theoretical methodology is described that combines stress determination using a finite element method with experimental determinations of the requisite fracture parameters, leading to the prediction of structural lifetimes. The stresses for an assumed geometry will be presented and com-bined with the fracture parameters needed to describe the behavior of the glass. These parameters include measures of the strength and strength distribution as well as the material's sensitivity to the service environ-ment. A preliminary stress-lifetime diagram for the material has been created and compared to the results of the finite element model.

101,420 PB91-187617 PC A06/MF A01 National Inst. of Standards and Technology, Gaithersburg, MD.

Journal of Research of the National Institute of Standards and Technology, March-April 1991. Volume 96, Number 2.

1991, 109p Also available from Supt. of Docs. as SN703-027-00039-3. See also PB91-187625 through PB91-187682 and PB91-184953. Library of Congress catalog card no. 89-656121.

Keywords: \*Photodiodes, Dimensional measurement, Particle size, Microsphere, Gel permeation chromatography, Light scattering, Molecular weight, Potassium chloride, Standards, Dental caries, Optical communication, Standard reference materials, Electrolytic conductivity, Bidirectional scattering distribution function.

Contents:

Linearity of a Silicon Photodiode at 30 MHz and Its Effect on Heterodyne Measurements; Use of the Electrostatic Classification Method to Size 0.1 micrometer SRM Particles--A Feasibility Study;

A Multiple Variable-Angle Light Scattering Detector for Gel Permeation Chromatography; Proposed New Electrolytic Conductivity Primary Standards for KCI Solutions;

Digital Image Analysis Assisted Microradiography--Measurement of Mineral Content of Caries Lesions in Teeth; Bidirectional Scattering Distribution Function

(BSDF)--A Systematized Bibliography; Limited International Intercomparison of Responsivity Scales at Fiber Optic Wavelengths.

PB91-187674

(Order as PB91-187617, PC A06/MF A01) National Inst. of Standards and Technology, Gaithersburg, MD.

Bidirectional Scattering Distribution Function (BSDF): A Systematized Bibliography.
C. Asmail. 1991, 9p

Included in Jnl. of Research of the National Institute of Standards and Technology, v96 n2 p215-223 Mar/Apr

Keywords: \*Light scattering, \*Bibliographies, Distribution functions, Inverse scattering, Specular reflection, Diffuse reflection, Surface properties, Polarization, \*BSDF(Bidirectional Scattering Distribution Function), \*Bidirectional scattering distribution function.

In conjunction with the development of a bidirectional scattering metrology project, a large number of papers pertaining to the theory and measurement of bidirectional scattering from optical surfaces were collected and categorized. The collection includes papers that deal with various aspects of the bidirectional scattering distribution function (BSDF), its measurement, interpretation, use, and implications. Each paper is classified in one or more subject categories on the basis of its technical content. The subject categories are in-cluded just to serve as a key to the most salient characteristics of each paper cited. Because of the interest in the field, the bibliography is being published as a service to the public.

101.422 PB91-189332 Not available NTIS National Inst. of Standards and Technology (IMSE), Gaithersburg, MD. Ceramics Div. Refractive Index Gratings in Rare-Earth-Doped Al-

kaline Earth Glasses.

Final rept. V. A. French, R. C. Powell, D. H. Blackburn, and D. C. Cranmer. 1991, 5p Sponsored by Army Research Office, Research Trian-

gle Park, NC. Pub. in Jnl. of Applied Physics 69, n2 p913-917, 15 Jan

Keywords: \*Gratings, Laser applications, Refractive index, Doped materials, Europium ions, Silicates, Glass, Reprints.

Four-wave-mixing techniques were used to produce permanent laser-induced refractive index gratings in Eu(3+)-doped silicate glasses. The gratings are associated with a thermally induced change in the local glass structure at the site of the Eu(3+) ions, leading to a double-minimum potential well for the electronic energy levels of the Eu(3+) ions. The effects on the characteristics of the permanent laser-induced gratings produced by changing the divalent modifier ions of the glass host are reported, and a theoretical model is presented to explain the physical origin of the change in the refractive index of the material.

PB91-189738 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Electricity Div. Effects of Colored Pump Noise on Intensity Corre-

lations of a Single Mode Dye Laser.

Final rept.
P. D. Lett, and E. C. Gage. 1989, 7p
Pub. in Physical Review A 39, n3 p1193-1199, 1 Feb

Keywords: \*Dye lasers, Optical pumping, Quantum optics, Langevin equation, White noise, Intensity, Reprints.

Recent theoretical analyses of the single mode laser with colored noise pump fluctuations have allowed the detailed prediction of the short-time behavior of the in-

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tensity autocorrelations of such a laser. In particular, a rounding-off of the intensity correlation function on the time scale of the correlation time of the pump fluctuations has been predicted. The authors present results from experiments performed on a single mode dye laser system that clearly confirm these predictions. Numerical simulations of the laser Langevin equations including the colored noise pump fluctuations are used to fit the experimental results.

101,424 PB91-189803 Not available NTIS Not available NTIS
National Inst. of Standards and Technology (NML),
Gaithersburg, MD. Molecular Spectroscopy Div.
Fourier Transform Infrared Spectroscopy at the
NIST: High Temperature Molecules and Atmos-

pheric Molecules. Final rept.

Piliarrepi.
A. G. Maki. 1989, 4p
Pub. in Proceedings of High Resolution Fourier Transform Spectroscopy Topical Meeting, Santa Fe, NM., February 13-15, 1989, p98-101.

Keywords: \*Fourier spectroscopy, \*Molecular spectroscopy, \*Infrared spectroscopy, Atmospheric chemistry, Air pollution, High temperature, Infrared instruments, Calibration, Reprints, US NIST

The paper gives some of the interesting results from three projects that involve Fourier Transform Spectroscopy (FTS) measurements, studies of molecules involved in atmospheric chemistry, high temperature studies, and the compilation of data for wavenumber calibration of infrared instrumentation. Earlier work on these projects was conducted with a tunable diode laser, now many of the measurements are made with a FTS spectrometer. The FTS instrument is not as sensitive as the diode laser spectrometer, nor does it give as high resolution, but it has the advantage of conveniently and quickly giving broad band spectra with thousands of absorption lines.

101,425 PB91-195644 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Radiometric Physics Div.
Roughened Quartz Surfaces and Teflon as Small-Angle Diffusers and Depolarizers between 200 and

Final rept.

R. D. Saunders, and H. J. Kostkowski. 1989, 4p Pub. in Applied Optics 28, n15 p3242-3245 1989

Keywords: \*Spectroradiometers, \*Diffusers, Rocketborne instruments, Near ultraviolet radiation, Small angle scattering, Depolarization, Quartz, Teflon, Reprints, \*Depolarizers.

Laboratory tests of transmission diffusers are reported for quartz and teflon. These tests were conducted in order to select transmission diffusers for the NOAA rocket-flight UV spectroradiometers.

101,426 PB91-203042 Not available NTIS National Bureau of Standards (IMSE), Gaithersburg, MD. Ceramics Div.

Alternate Representation of Prism Refraction for

Light Incident at the Brewster Angle. Final rept.

A. Feldman. 1988, 2p

Pub. in Applied Optics 27, n22 p4608-4609 1988.

Keywords: \*Optics, \*Optical materials, \*Prismatic bodies, \*Brewster angle, Graphs(Charts), Visible radiation, Reprints.

An alternate representation of prism refraction provides a convenient context for solving the problem of a beam incident on a wedged plate at the Brewster angle and allows for a graphical solution based on a simple geometric construction.

101,427 PB91-203109 PB91-203109 Not available NTIS National Inst. of Standards and Technology (NEL), Boulder, CO. Electromagnetic Technology Div. Frequency Stabilization of a Tunable Erbium-Doped Fiber Laser.

Final rept.

S. L. Gilbert. 1991, 3p Sponsored by Naval Sea Systems Command, Wash-

Pub. in Optics Letters 16, n3 p150-152, 1 Feb 91.

Keywords: Near infrared radiation, Optical communication, Frequency standards, Frequency stability, Infrared lasers, Tunable lasers, Acetylene, Reprints, \*Erbium lasers, Fiber lasers, Wavelength standards.

A single-frequency Er-doped fiber laser that is tunable from 1.52 to 1.58 micrometers has been constructed. The laser linewidth was determined to be less than 1.6 MHz FWHM by observing the spectrum of the beat between the fiber laser and a 1.523 micrometer He-Ne laser. The frequency of the fiber laser was locked to several absorption lines of acetylene near 1.53 mi-crometers. The research demonstrates the inherent stability of fiber lasers and their potential for use in a wavelength standard for optical communications.

101,428 PB91-203158 Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Precision Engineering Div.

Note on the Precision Cementing of Small Optical Components.

Final rept.
A. W. Hartman. 1988, 2p
Pub. in Review of Scientific Instruments 59, n12 p2617-2618 1988.

Keywords: \*Optical equipment, \*Cementing, Alignment, Substrates, Precision, Shrinkage, Reprints.

When optical or mechanical components are cemented to a substrate that exhibits errors in surface figure or tilt angle, the possibility exists that these errors will propagate to the work piece. If the cement layer thickness shrinks by a given fraction p during setting of the cement, the error propagation will occur at the same fraction causing losses in flatness, tilt angle, etc. These losses can be reduced to near harmless levels by adopting a two-stage cementing process, involving an intermediate substrate.

101,429 PB91-203802 Not available NTIS National Inst. of Standards and Technology (NEL), Boulder, CO. Electromagnetic Fields Div.
New Triple Correlator Design for the Measurement of Ultrashort Laser Pulses.

N. G. Paulter, and A. K. Majumdar. 1991, 6p Pub. in Optics Communications 81, n1-2 p95-100, 1

Keywords: \*Optical correlators, \*Correlators, Optical measurement, Laser radiation, Light pulses, Nonlinear optics, Design, Reprints.

A measurement device, a triple correlator, is proposed for the characterization of ultrashort optical pulses. The proposed triple correlator uses two consecutive nonlinear optical interactions, a sum frequency generation followed by a difference frequency generation, to produce a triple correlation output at the same optical frequencies as the input pulse. Phase matching for the triple correlator is greatly simplified by using the given design. The operation of the triple correlator is described, and examples of expected output signals are given. The reconstructed optical pulse is quite insensitive to noise, as shown by computer simulations.

PR91-203984 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Atomic and Plasma Radiation Div. Precise Laser Wavelength Measurements: What Can We Learn from Classical Spectroscopy. Final rept.

C. J. Sansonetti. 1989, 6p Pub. in Proceedings of International Laser Science Conference (4th), Advances in Laser Science IV, Atlanta, GA., 1988, p548-553 1989.

Keywords: \*Dye lasers, \*Laser radiation, \*Wave-meters, Fabry Perot interferometers, Continuous wave lasers, Fourier spectrometers, Reprints, \*Wavelength measurement.

The wavelengths of cw dye lasers are typically measured using Michelson wavemeters, but the absolute accuracy of such instruments is limited by their sensitivity to alignment of the laser beams. This systematic problem can be largely eliminated by diffusely scattering the beams and using classical spectroscopic methods to measure the wavelength. We have developed a laser wavemeter, based on a static Fabry-Perot interferometer, with an accuracy of a few parts in a billion and an update rate of about 2 Hz. The system is insensitive to the alignment and collimation of the incoming laser beams. The potential for a more precise wavemeter based on techniques of Fourier transform spectroscopy is also considered.

PB91-204016 Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Quantum Physics Div. Production and Diagnosis of a Highly Spin-Polar-

ized Na Beam.

Final rept.
G. W. Schinn, X. L. Han, and A. Gallagher. 1991, 5p
Contract DE-FG02-87ER13720

Sponsored by Department of Energy, Washington, DC. Office of Basic Energy Sciences.
Pub. in Jnl. of the Optical Society of America B 8, n1

p169-173 Jan 91.

Keywords: \*Sodium, \*Optical pumping, Laser induced fluorescence, Polarization(Spin alignment), Atomic beams, Reprints.

The authors describe optically pumping a beam of sodium atoms to >96% m(s) and >92% m(s), m(l) state selection. For the optical pumping both ground hyperfine states are pumped, using single-mode cw dye-laser radiation tuned to the triplet S(1/2)-triplet P(1/2) transition that is phase modulated in a LiTaO3 crystal to produce first-order sidebands at approxi-mately the 1772-MHz hyperfine splitting of the ground state. The z-directed optical pumping is performed in a z-directed magnetic field of (about) 5 G. The state-selected atoms then move, in (about) 1 cm, into an (about) 200 G, z-directed field. The downstream probe laser beam is scanned through the triplet S(1/2) (m(s), m(l) -> triplet P(3/2) (m'(s), m(l)) transitions, which are spectroscopically resolved at 200 G, and the fluorescence intensities portray the residual populations in each of the eight triplet S(1/2) states.

101.432

PB91-204180 Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Quantum Physics Div. Correlated Spontaneous Emission in a Zeeman

Laser.

Final rept.
M. P. Winters, and J. L. Hall. 1990, 9p
Contract N00014-89-J-1227, Grant NSF-PHY86-

See also PB91-175596. Sponsored by Office of Naval Research, Arlington, VA., and National Science Foundation, Washington, DC.
Pub. in New Frontiers in Quantum Electrodynamics

and Quantum Optics, p193-201 1990.

Keywords: Gravitational wave detectors, Spontaneous emission, High sensitivity, Reprints, \*Zeeman lasers, Correlated emission lasers, Laser interferometers, Squeezed states.

In recent years there has been great interest in the development of high sensitivity laser interferometers for use in the detection of gravitational waves. Ordinarily, the sensitivity of these devices is limited by quantum fluctuations that take the form of shot noise in passive interferometers and spontaneous emission noise in active interferometers. Proposals for increasing the sensitivity of these interferometers include squeezed states for passive devices and the correlated emission laser (CEL) for active devices. Generation of squeezed states has now been demonstrated by several groups and it is the purpose of the article to describe an experimental investigation of the CEL.

101,433

Not available NTIS PB91-237065 National Inst. of Standards and Technology (NML), Gaithersburg, MD. Atomic and Plasma Radiation Div. Exploding Foil Photoionization X-ray Laser. Final rept.

P. D. Morley, and J. Sugar. 1988, 4p Pub. in Physical Review A 38, n6 p3139-3142 1988.

Keywords: \*X ray lasers, Multicharged ions, Iodine ions, Soft x rays, Photoionization, Inner-shell ionization, Reprints, \*Copper-like ions, Exploding foils.

By combining the techniques of exploding foils and inner-shell photoionization, it is predicted that lasing can occur for x-rays less than 50 A. As an example, the authors work out the case for Cu-like iodine (I(24 +)) which should lase on the 3d(10)4p - 3d(9)4s(2) doublet calculated at 24.565 A and 26.026 A with integrated line intensities comparable to the selenium x-ray laser.

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101,434

PB91-237156 Not available NTIS National Inst. of Standards and Technology (EEEL), Boulder, CO. Electromagnetic Fields Div.

New Triple Correlation Technique for Measuring Ultrashort Laser Pulses.

Final rept.

N. G. Paulter, and A. Majumdar. 1991, 12p

See also PB91-203802.

Pub. in Review of Scientific Instruments 62, n3 p567-578 Mar 91.

Keywords: \*Laser radiation, \*Light pulses, Picosecond pulses, Nonlinear optics, Optical measurement, Reprints, Triple correlation method.

A new triple correlation technique for measuring the complete intensity profile of ultrashort optical pulses is described. The triple correlation preserves the phase information of the input pulse so that a reconstruction of the triply correlated signal will provide a unique re-construction of the input. The new technique de-scribed here uses two second-order, nonlinear optical interactions for the generation of a triply correlated signal. A derivation of the measured triple-correlation signal and the pulse reconstruction is given. The effects of noise on the measured signal are also exam-

101,435

PB92-102185 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Radiometric Physics Div. LBIR Facility User Handbook.

Final rept.

R. U. Datla, S. C. Ebner, J. Proctor, and A. C. Parr. Jun 91, 31p NIST/HB-147

Sponsored by Army Strategic Defense Command,

Keywords: \*Research facilities, \*Handbooks, Blackbody radiation, Clean rooms, Standards, \*Low Background Infrared Calibration Facility(LBIR), \*LBIR facility, Absolute cryogenic radiometer, US NIST.

A handbook has been prepared to aid prospective users of NIST's Low Background Infrared Calibration Facility(LBIR). A detailed overview of the facility is given, including directions to the NIST site and places to stay. The sponsorship of the facility by the Strategic Defense Command to serve the community using blackbody sources in a cryogenic environment is stated in the introduction. The vacuum and cryogenic hardware associated with the facility is discussed in detail, as well as procedures the user must follow regarding clean room practice, vacuum compatibility, and electrical hookup. Much discussion is also given to Absolute Cryogenic Radiometer (ACR) which serves as the standard detector for the system. An electrical substitution radiometer, the ACR measures the total flux emitted from a blackbody.

101,436

PB92-116532 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Precision Engineering Div. Light-Scattering Measurement of the RMS Slopes

of Rough Surfaces.

Final rept. L. X. Cao, T. V. Vorburger, A. G. Lieberman, and T. R. Lettieri. 1991, 7p

Pub. in Applied Optics 30, n22 p3221-3227, 1 Aug 91.

Keywords: \*Surface roughness, \*Optical measurement, Laser applications, Light scattering, Metrology, Texture, Slope, Reprints.

Angle-resolved light scattering (ARLS) is used to estimate the root-mean-square (rms) slopes of rough surfaces having a well-defined lay, and the effect on slope measurements caused by changing the angles of incidence and scattering is investigated. The ARLS patterns are taken with the Detector Array for Laser Light Angular Scattering (Dallas) research instrument, and the rms slopes are obtained from the angular widths of these patterns. In general, it was found that the angular width, and thus the estimated rms slope, is surpris-ingly insensitive to relatively large changes in both the incident and scattering angles of light. These results are independent of surface material and are valid for both sinusoidal and random rough surface with lay. The principles, experiments, analyses, and conclusions involved in using ARLS to estimate rms surface slopes are described.

101,437 PB92-116888 Not available NTIS National Inst. of Standards and Technology (EEEL), Boulder, CO. Electromagnetic Fields Div.

Diffraction by a Half-Plane in a Lossy Medium.

Final rept. D. A. Hill. 1991, 3p

Sponsored by Army Belvoir Research and Development Center, Fort Belvoir, VA.
Pub. in Jnl. of Applied Physics 69, n12 p8405-8407, 15

Keywords: \*Wave diffraction, \*Diffraction, Plane waves, Fresnel integrals, Fresnel zones, Polarization, Remote sensing, Reprints.

The classical problem of plane-wave diffraction by half-plane is extended to allow for loss in the surround-ing medium. The loss causes the arguments of the in-tegral functions to become complex. Numerical results show that the relative importance of the edge-diffract-ed field decreases as the loss is increased. This effect is important in interpreting the effects of off-path scat-terers in remote sensing of lossy media. The results for both electric and magnetic polarizations are in qualitative agreement with previous results based on the Kirchhoff approximation.

101.438

PB92-116896 Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Time and Frequency Div.

CW Dye Lasers. Final rept.

L. Hollberg. 1990, 54p Pub. in Dye Laser Principles with Applications, Chapter 5, p185-238 1990.

Keywords: \*Continuous wave lasers, \*Dye lasers, Historical aspects, Frequency control, Performance, Design, Theory, Reprints.

The chapter describes the principles, construction, performance, and some of the theory of Cw dye lasers. It briefly reviews the history of Cw dye laser development and also the modern frequency control technol-

101,439

PB92-116904 Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Time and Frequency Div.

Diode Lasers and Their Application to Spectrosco-

py. Final rept.

L. Hollberg, 1990, 9p

Pub. in Applied Laser Spectroscopy, p117-125 1990.

Keywords: \*Semiconductor lasers, \*Spectroscopy, Semiconductor diodes, Reviews, Uses, Reprints.

The paper is a brief review of lasers and their application to spectroscopy.

101,440 PB92-126531 PC A08/MF A02 National Inst. of Standards and Technology (EEEL), Boulder, CO. Electromagnetic Technology Div.

Modified Airy Function and WKB Solutions to the

Wave Equation.

A. K. Ghatak, R. L. Gallawa, and I. C. Goyal. Nov 91, 175p NIST/MONO-176 Also available from Supt. of Docs. See also PB91-236752. Prepared in cooperation with Indian Inst. of Tech., New Delhi. Dept. of Physics.

Keywords: \*Optical waveguides, Optical fibers, Wave equations, Integrated optics, WKB approximation, Reprints, Airy Functions.

The WKB method has served in problems of quantum mechanics and nonuniform optical waveguides, the discipline treated in the monograph. The monograph discusses the WKB and the Modified Airy Function (MAF) methods in considerable detail, to the end that the reader gains an appreciation of the strengths and the reader gains an appreciation of the strengths and appreciation of the strengths and the strengths are stre weaknesses of each. The authors treat eigenvalue problems as well as initial value problems. The two methods could be illustrated via any of several disciplines, but they chose to use problems that are of current interest to the optical waveguide community. They have also used Schrodinger's equation for typical potential well problems to further illustrate the method. Both the wave functions and the eigenvalues are found. They have also included several exercises, to be solved by the reader. They give several examples to illustrate the method for problems of interest in optical telecommunications devices.

## Plasma Physics

101,441 AD-A227 656/6 PC A02/MF A01 National Inst. of Standards and Technology, Boulder,

Liquid and Solid Ion Plasmas.

Annual rept. 1 Oct 89-31 Sep 90.

D. J. Wineland, and J. J. Bollinger. 15 Sep 90, 10p. Contract N00014-89-F-0020

Keywords: Angular momentum, Cooling, Coupling(Interaction), Radiative transfer, Distribution functions, Flectromagnetic fields, Images, lons, Laser applications, \*Plasmas(Physics), Spatial distribution, Spectroscopy, Temperature, Velocity, Penning Traps, Laser Cooling.

Atomic ions which are stored in electromagnetic fields are an example of nonneutral plasmas. Laser techniques allow control of plasma angular momentum and provide plasma cooling to temperatures much less than 1K. Using imaging techniques, plasma spatial information is achieved. Laser spectroscopic techniques allow measurement of plasma velocity distribution functions. Liquid and solid behavior of ion plasmas is studied. Keywords: Nonneutral plasma; One component plasma; Strongly coupled plasma; Liquid and solid plasma, Plasma distribution functions; Penning trap; Laser cooling. (jhd)

101.442

PB91-147504 Not available NTIS
National Inst. of Standards and Technology (NML),
Gaithersburg, MD. Atomic and Plasma Radiation Div.
Overview of the Ion Dynamic Effect in Line Broadening, and a Generalization of the Unified Theory.

Final rept.
D. E. Kelleher, D. H. Oza, J. Cooper, and R. L. Greene. 1990, 7p
Pub. in Jnl. of Quantitative Spectroscopy and Radiative Transfer 44, n1 p101-107 1990.

Keywords: \*Thermal plasmas, \*Line broadening, Computation, Reprints, Ion dynamics.

The authors present a brief overview of the collisional broadening of hydrogenic radiators in thermal plasmas. Their focus is on lines with unshifted central components, particularly the alpha lines (Delta = 1), for which ion motion effects can be very large. The calculations span a wide range of electron densities, temperatures, and radiator - ion perturber reduced masses mu. The computations were made using a numerical simulation approach. Numerical methods have proven necessary to deal with the overlapping strong collisions of different ion perturbers. Most current analytical methods, such as the unified theory, are not valid when strong collisions overlap, as is often the case with ion perturbers.

101,443

PB91-158618 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Radiometric Physics Div.

Relative Populations of Excited Levels within the Ground Configuration of Si-Like Cu, Zn, Ge, and Se lons.

Final rept. R. U. Dalta, J. R. Roberts, and A. K. Bhatia. 1991, 4p

Contract DE-EA-77-A-01-6010 Sponsored by Department of Energy, Washington, DC. Pub. in Physical Review A 43, n2 p1110-1113, 15 Jan

Keywords: \*Copper ions, \*Zinc ions, \*Germanium ions, \*Selenium ions, Multicharged ions, Excited states, TEXT devices, M1-transitions, Electron collisions, Reprints, Proton collisions.

Populations of 3p(2) singlet D(2), triplet P(1), triplet P(2) levels in Si-like Cu, Zn, Ge, and Se ions have been deduced from the measurements of absolute intensities of magnetic dipole transitions within the 3s(2) 3p(2) ground configuration. Observations have been made in the Texas Experimental Tokamak (TEXT). The measured population ratios are compared with

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theoretical calculations based on the distorted-wave approximation for the electron collisions and a semiclassical approximation for the proton collisions. The observed deviation from the statistical distribution for the excited-level populations within the ground config-uration along the silicon isoelectronic sequence is in agreement with theoretical prediction.

101,444 PB92-117225 Not available NTIS National Inst. of Standards and Technology (EEEL), Gaithersburg, MD. Electricity Div.

Off-Axis Measurements of Ion Kinetic Energies in RF Plasmas. Final rept.

S. B. Radovanov, J. K. Olthoff, and R. J. Van Brunt. 1991, 2p

Sponsored by SEMATECH, Austin, TX.

Pub. in Proceedings of International Conference on Phenomena in Ionized Gases (20th), Barga, Italy, July 8-12, 1991, p835-836.

Keywords: \*Argon plasma, Argon ions, Kinetic energy, Gas discharges, RF systems, Reprints, Reference

lon kinetic energy distributions are presented for argon plasmas in the GEC RF reference cell and are compared with other previous measurements.

101,445

PB92-126473 PC A04/MF A01 Mational Inst. of Standards and Technology (NML), Gaithersburg, MD. Ionizing Radiation Div. Mass Energy-Transfer and Mass Energy-Absorp-

tion Coefficients, Including In-Flight Positron Annihilation for Photon Energies 1 keV to 100 MeV.
P. D. Higgins, F. H. Attix, J. H. Hubbell, S. M. Seltzer,
M. J. Berger, and C. H. Sibata. Nov 91, 70p NISTIR-4680

See also PB87-116141, PB88-109830, UCRL-50400-V6-REV-2 and UCRL-50174-SEC-2-R1. Prepared in cooperation with Cleveland Clinic Foundation, OH. Dept. of Radiation Therapy, and Wisconsin Univ.-Madison. Dept. of Medical Physics.

Keywords: \*Energy transfer, \*Photon cross sections, \*Energy absorption, Scattering, Computation, Pair production, X rays, Gamma rays, Bremmstrahlung, Photoelectric emission, Irradiation, Corrections, Radiography, Positrons.

Mass energy-transfer (Mu(sub u)/Rho) and mass energy-absorption coefficients (Mu(sub en)/Rho) are tabulated in units of (sqcm/g) for photon energies be-tween 1 keV and 100 MeV for 29 elements (Z = 1-92), and 14 mixtures and compounds of general dosimetric interest. Cross sections for photo-effect, incoherent scattering, pair and triplet production are those com-piled or generated by the National Institute of Stand-ards and Technology (NIST) (formerly the National Bureau of Standards). Corrections are included for in-flight positron annihilation, previously not applied in NIST calculations for energies above 10 MeV.

## Radiofrequency Waves

PB91-203505 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Precision Engineering Div.

Computed Fields Near the Edge of a Dielectric

Final rept.

E. Marx. 1990, 5p Pub. in IEEE (Institute of Electrical and Electronics Engineers) Transactions on Antennas and Propagation 38, n9 p1438-1442 Sep 90.

Keywords: \*Electromagnetic scattering, Electromagnetic fields, Integral equations, Edges, Reprints, Dielectric wedges.

The behavior of the electromagnetic field near the edge of an infinite sharp dielectric wedge has not been unequivocally established, and a numerical experi-ment is performed to learn about this behavior. The fields scattered by a finite wedge are determined by solving an integral equation. The fields near the edge of the wedge are computed from a boundary function by integration. The theory of the fields near the edge of

the dielectric wedge appears to imply that some of the components diverge, but the analysis is based on a power series expansion that has not been shown to exist. The numerical experiment shows that the behavior of the fields near the edge does not follow the expected behavior. The problem of the perfectly conducting wedge is well understood and is used here to verify the numerical methods.

101,447 PB91-203513 Not available NTIS

National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Precision Engineering Div. Scattering by an Arbitrary Cylinder at a Plane

Final rept.
E. Marx. 1989, 10p
Pub. in IEEE (Institute of Electrical and Electronics Engineers) Transactions on Antennas and Propagation 37, n5 p619-628 1989.

Keywords: \*Electromagnetic scattering, Radar cross sections, Maxwells equations, Integral equations, Plane waves, Interfaces, Cylinders, Dielectrics, Re-

The problem of the determination of the fields scattered by an infinite cylinder of arbitrary cross section located at the interface between two semi-infinite media is reduced to the solution of integral equations for unknown functions defined on the boundaries. These boundary functions are chosen so as to minimize their number. The incident field is that of a plane monochromatic wave. The derivation of the integral equations is given for the TE mode for a dielectric cylinder and for a perfectly conducting cylinder. The exact electromagnetic fields are obtained from the solutions of the integral equations by integration, and the radar cross section can be computed from the far-field approximation. Sample outputs of the computer programs that implement the solution are shown.

#### Solid State Physics

101,448 AD-A231 818/6 PC A02/MF A01 National Inst. of Standards and Technology (IMSE), Gaithersburg, MD. Ceramics Div. Influence of Filament Geometry on Hot Filament

Growth of Diamond Films.

Technical rept. E. N. Farabaugh, A. Felfman, and L. Robins. 5 Feb 91, 8p Rept no. TR-1 Contract N00014-90-F-0011

Keywords: Filaments, Silicon, Single crystals, Substrates, \*Diamond films.

The influence of filament geometry on growth rate and morphology has been observed on diamond films deposited on single crystal silicon substrates in a hot filament CVD reactor. Single and dual helical W filaments having 5, 10, or 15 turns and CH4: H2 ratios of 0.25%-1.00% were used. With single filaments the deposition rate was approximately proportional to the number of turns in the filaments produced lower deposition rates, compared to single filaments for depositions carried out at the same CH4:H2 of 0.5%. Employing dual filaments doubled the area of uniform growth. Faceting of our films changed from (111) to (100), as the CH4:H2 ratio was increased.

AD-A243 093/2 PC A03/MF A01 National Inst. of Standards and Technology, Gaithers-

High Resolution Electron Microscopy of Diamond Film Growth Defects and their Interactions. Technical rept.

D. Shechtman, E. N. Farabaugh, L. H. Robins, and A. Feldman. 25 Sep 91, 25p Contract N00014-90-F-0011

Keywords: Angles, Crystal growth, Crystals, Defects(Materials), Density, Diamonds, Electron microscopy, Grain size, High rate, High resolution, Locus, Microstructure, Sites Microstructure, Nucleation, Sites, Twinning(Crystallography), \*Diamond films, Chemical vapor deposition.

High resolution electron microscopy of plasma-assisted chemical vapor deposition (CVD) diamond films

was performed. The film was fine grained with a grain size of the order of 0.1 micrometer. Several features of the microstructure were studied and their importance to the understanding of the diamond film growth was evaluated. The observation include: 1. Twinning density rises as a function of the distance from the center of the crystal. 2. The twins have an important role in the rapid growth of this kind of film. The reentrant angle between intersecting twins serves as a nucleation site for the growth of new (111) planes. 3. The center point of a twin quintuplet has five reentrant angles and thus serves as a preferred nucleation site for new planes as the crystal grows. 4. Misfit boundaries, being the locus of intersection points of the growing planes on two adjacent twins can serve as an indicator for the local crystal growth direction. The central nucleation site serve as an indicator for the local crystal growth direction. The central nucleation site for the growing planes can thus be traced back in many cases to a quintuplet twin point.

101,450 AD-A243 096/5 PC A03/MF A01 National Inst. of Standards and Technology, Gaithersburg, MD.

Transmission Electron Microscopy of the CVD Diamond Film/Substrate Interface.

Technical rept. D. Shechtman. 27 Sep 91, 14p Contract N00014-90-F-0011

Keywords: Diamonds, Electrical properties, Germanium, Grain boundaries, Interfaces, Mechanical properties, Migration, Semiconductors, Silicon, Substrates, \*Diamond films, Transmission electron microscopy, Chemical vapor deposition.

The structure of grain boundaries in the diamond lattice, and twin boundaries as a special case, received considerable attention in over thirty years. This is mainly due to the importance of defects in silicon and germanium to their usefulness as efficient semiconductors. Twin boundaries have equal importance to various properties of diamond films. Electrical and mechanical properties as well as migration mechanisms are all affected by the twin boundaries and their structure. The ever presence of twins in CVD diamond films makes their study even more important compared to semiconductors which can be grown without boundaries. The purpose of the study reported here is, therefore, to investigate the crystallography of twin boundaries which form in chemical vapor deposited (CVD) diamond films, and to compare them to the ones which were found in silicon and in germanium.

101,451 AD-A243 220/1 AD-A243 220/1 PC A03/MF A01 National Inst. of Standards and Technology, Gaithersburg, MD.

Spatially and Spectrally Resolved Cathodoluminescence Measurements of CVD-Grown Diamond Particles and Films.

Technical rept.
L. H. Robins, E. N. Farabaugh, and A. Feldman. 27
Sep 91, 15p Rept no. NIST-TR-6
Contract N00014-90-F-0011

Keywords: \*Cathodoluminescence. Concentration(Composition), Cross sections, Depth, Gradients, Impurities, Interfaces, Low temperature, Lu-minescence, Measurement, Particles, Polycrystalline, Recombination reactions, Silicon, Spatial distribution, Substrates, \*Diamonds, Color centers, Crystal struc-ture, Chemical vapor deposition, \*Diamond films.

Spatially and spectrally resolved cathodoluminescence (CL) was used to investigate the spatial distribution of luminescence centers in CVD-grown diamond particles and polycrystalline films. For single particles grown at a low substrate temperature (nominally 650 C), one of the two most intense CL bands, the 2.156 eV band, was found to be associated with (111) facets. The CL image of the other intense band, the 2.85 eV band, showed considerable particle-to-particle variation among the same particles. The images of the 2.156 eV and 2.85 eV CL bands were found to have a complementary relationship for some particles. A model of competing recombination centers is proposed to help explain these results. Cross-sectional measurements of the CL spectra of polycrystalline films on silicon showed that the intensity of a silicon-impurity-related CL band decreases with increasing distance from the film-substrate interface. This depth variation is interpreted as due to a silicon impurity con-centration gradient.

101,452 DE91016275 PC A03/MF A01 National Inst. of Standards and Technology, Boulder,

Integrity tests for high-(Tc) and conventional critical-current measurements systems.

L. F. Goodrich, and S. L. Bray. 1989, 15p CONF-

890701-30

Contract Al01-86ER52132

International cryogenic materials conference, Los Angeles, CA (United States), 24-28 Jul 1989. Sponsored by Department of Energy, Washington, DC.

Keywords: \*Superconductors, Electric Impedance, Electrical Testing, High-Tc Superconductors, Measuring Methods, Simulation, Meetings, EDB/420500, EDB/360204.

A set of simple procedures that will test the integrity of measurement systems used for critical-current determinations on high-(Tc) and conventional superconductors has been developed. These tests include a finite resistance, a zero resistance, and a superconductor voltage-current simulator. In the measurement of the critical current, voltage sensitivity is a key factor. The zero resistance test is the most effective test to detect the presence of interfering voltages such as ground loop or common-mode voltages and will determine the voltage sensitivity limit of a measurement system. 5 refs., 3 figs.

101,453 N91-20208/5

(Order as N91-20207/7, PC A05/MF A01) National Bureau of Standards (IMSE), Gaithersburg,

High T(sub C) Superconductors: Are They Magnet-

R. D. Shull. Jan 90, 5p

In NASA, Langley Research Center, National Educators' Workshop: Update 1988. Standard Experiments in Engineering Materials Science and Technology p 1-

Keywords: Experimentation, \*High temperature super-conductors, Magnetic properties, Oxides, Procedures, Transition temperature, \*Yttrium barium cuprates.

The objective is to demonstrate the magnetic characteristics of the new superconducting oxides with transition temperatures above liquid nitrogen temperature (77 K). The first task was to find out whether YBa2Cu3O7-x is magnetic at liquid nitrogen temperature, and if so, what the sign of its magnetic susceptibility is. Details of the experimental procedure are given.

PATENT-4 954 481 Not available NTIS Department of Commerce, Washington, DC. Superconductor-Polymer Composites. Patent.

A. S. DeReggi, C. K. Chiang, and G. T. Davis. Filed 29 Dec 88, patented 4 Sep 90, 2p PB91-176032, PAT-APPL-7-292 601

This Government-owned invention available for U.S. licensing and, possibly, for foreign licensing. Copy of patent available Commissioner of Patents, Washington, DC 20231 \$1.50.

Keywords: \*Superconducting films, \*Polymer matrix composites, \*Particulate composites, \*Patents, Rare earth alloys, Cuprates, Barium oxides, Thermoplastic resins, Polymeric films, Thin films, PAT-CL-505-1, Vinylidene fluoride resins.

Superconductor-polymer composite materials comprise a matrix formed of a thermoplastic polymer and a superconductor powder dispersed in the matrix. The superconductor powder preferably has a composition RBa2Cu3O(7-x) wherein R is a rare earth metal and x is less than or equal to 1. The thermoplastic polymer matrix comprises a vinylidene fluoride homopolymer or copolymer. The composite materials may be formed as shaped products, sheets or films.

101,455 PB91-133827 Not available NTIS National Inst. of Standards and Technology (NEL), Boulder, CO. Electromagnetic Technology Div. Current Supply for High-T(sub c) Superconductor Testing. Final rept.

S. L. Bray, and L. F. Goodrich. 1990, 4p Sponsored by Department of Energy, Washington, DC.

Pub. in Meas. Sci. Technol. 1, p491-494 1990.

Keywords: \*Superconductors, Electrical measurement, Direct current, Power supplies, Design, Reprints, \*High temperature superconductors, \*Critical current,

Precise and accurate measurements of the DC critical current of high-T(c) superconductors often require a current supply that has high input-to-output isolation, high isolation from ground and low output ripple. Also, to ensure precise current control, the supply should have low current drift and its input-output characteristic should be linear. A design for a simple and inexpensive current supply that has these characteristics is presented. The primary power source is a 12 V wet-cell battery and the typical operating range is from 10 mA to 10 A. The supply's current ripple is <0.4 mA RMS over this operating range. At an output current of 5 A the current drift is <2%/h without a warm-up period. The maximum variation of the supply's output from linearity, over its full operating range is <5%.

101,456 PB91-133983 PB91-133983 Not available NTIS National Inst. of Standards and Technology (NEL),

Boulder, CO. Electromagnetic Technology Div.
Transport Critical Current of Aligned Polycrystalline Y1Ba2Cu3O7-delta and Evidence for a Nonweak-Linked Component of Intergranular Current Conduction.

J. W. Ekin, H. R. Hart, and A. R. Gaddipati. 1990, 11p

Sponsored by Department of Energy, Washington, DC., and Office of Naval Research, Arlington, VA. Pub. in Jnl. of Applied Physics 68, n5 p2285-2295, 1 Sep 90.

Keywords: \*Superconductors, \*Grain structure, Magnetic fields, Direct current, Polycrystalline, Alignment, Reprints, \*High temperature superconductors, \*Yttrium barium cuprates, \*Critical current, Weak links.

A study of grain alignment and its effect on the do transport critical current in fine-grained bulk Y1Ba2Cu3O(7-delta) is reported in magnetic fields from 0.0001 T to 26 T. The data clearly demonstrate that alignment alone significantly reduces the weak-link problem in fine-grained polycrystalline samples with low-aspect-ratio (4:1) grains (unlike melt-grown samples where there has been some ambiguity as to the relative importance of alignment versus large grain growth). Furthermore, the results provide strong evigrowth). Furthermore, the results provide strong evidence that there are two parallel components of inter-granular current conduction, one consisting of weak-linked material, the other behaving like intrinsic intragranular material that is not weak-linked. Field-cooled and force-free J(c) data are also presented, along with detailed measurements of the shapes of the voltagecurrent characteristics.

101,457 PB91-134056 Not available NTIS National Inst. of Standards and Technology (NEL), Boulder, CO. Electromagnetic Technology Div.
High T(sub c) Superconductors and the Critical
Current Measurement.

Final rept. L. F. Goodrich, and S. L. Bray. 1990, 11p Pub. in Cryogenics 30, p667-677 Aug 90.

\*Superconductors. Electrical measure-Kevwords: ment, Recommendations, Reprints, \*High temperature superconductors, \*Critical current, Interlaboratory comparisons.

With the introduction of high T(c) superconductors, a number of problems associated with critical current I(c) measurement have arisen. The existing I(c) measurement practices were developed and proved for low T(c) superconductors. There are substantial differences between the two classes of materials. When the ences between the two classes of materials. When the I(c) concept was casually extended to the high T(c) conductors, measurement inconsistency, ambiguity and, in some cases, invalidity followed. A discussion of the underlying philosophy of I(c) measurement is presented, and a number of measurement variables that can influence the measured I(c) are discussed. Many of the problems stem from inadequate reporting practices, and recommendations are given for improving measurement reports.

101,458 PB91-134148 Not available NTIS National Inst. of Standards and Technology (NEL), Boulder, CO. Electromagnetic Technology Div. Fundamental and Harmonic Susceptibilities of YBa2Cu3O7-delta.

Final rept.

T. Ishida, and R. B. Goldfarb. 1990, 12p Sponsored by Ministry of Education, Science and Culture, Tokyo (Japan).

Pub. in Physical Review B 41, n13 p8937-8948, 1 May

Keywords: \*Superconductors, Magnetic measurement, Magnetic fields, Magnetization, Reprints, \*High temperature superconductors, \*Magnetic susceptibility, \*Yttrium barium cuprates, Temperature depend-

The authors have examined the complex harmonic magnetic susceptibilities chi(sub n) of the sintered high-critical-temperature superconductor YBa2Cu3O(7-delta). The experimental variables for the measurements of chi(sub n) were the sample temperature, the ac magnetic field amplitude, frequency, and the magnitude of a superimposed dc field H(dc). Results are given.

101,459

PB91-134254 Not available NTIS National Inst. of Standards and Technology (IMSE), Boulder, CO. Fracture and Deformation Div.

Madelung Potentials and Valences in the Y1Ba2Cu3O7 Superconductor. Final rept.

H. Ledbetter, and M. Lei. 1990, 3p Pub. in Physica C 166, p483-485 1990.

Keywords: \*Superconductors, Valence, Reprints, \*High temperature superconductors, \*Yttrium barium cuprates. Ewald method.

Using Ewald's method, the authors calculated the ionsite potentials and Madelung energy of Y1Ba2Cu3O7(orthorhombic, Pmmm, No. 47). They considered the effects of copper-ion and oxygen-ion valences. Among seven suggested copper-oxygen ion-charge configurations, only two give a low electrostatic bonding energy to agree with oxygen vacancies on O(1) sites. Only one configuration gives a realistic bulk modulus. The authors perturbed this configuration by equalizing the Cu(1)-Cu(2) valences and introducing a hole into the CuO2 plane at the oxygen sites. This configuration also agrees well with observation.

101,460

PB91-134262 Not available NTIS National Inst. of Standards and Technology (IMSE), Boulder, CO. Fracture and Deformation Div.

Elastic Constants, Debye Temperatures, and Electron-Phonon Parameters of Superconducting Cuprates and Related Oxides.

Final rept. H. Ledbetter, M. Lei, and S. Kim. 1990, 10p Pub. in Phase Transitions 23, p61-70 1990.

Keywords: \*Superconductors, Strontium titanates, Barium titanates, Elastic properties, Electron phonon interactions, Bulk modulus, Reprints, \*High temperature superconductors, Lanthanum strontium cuprates, Yttrium barium cuprates, Lanthanum cuprates, Debye temperature, Kresin model, Born model.

Using both measurements and modeling, the authors studied the cohesive and related properties of several oxides. Superconducting oxides include La(1.85)Sr(0.15)CuO4, Y1Ba2Cu3)7, and (Bi-Pb)2Sr2Ca2Cu3O10. Related nonsuperconducting oxides include SrTiO3, BaTiO3, and La2CuO4. For these materials, the authors give the complete quasii-sotropic elastic constants corrected to the void-free state. From elastic constants and atomic volume, the authors caluclate Debye characteristic temperatures. The authors support their elastic-constant measure-ments with Born-model calculations of the bulk modu-

101,461 PB91-134270 Not available NTIS National Inst. of Standards and Technology (IMSE), Boulder, CO. Fracture and Deformation Div. Elastic Constants of Polycrystalline Bi-Pb-Sr-Ca-Cu-O Superconductor.

Final rept.
H. M. Ledbetter, S. A. Kim, R. B. Goldfarb, and K. Togano. 1989, 4p
Pub. in Physical Review B 39, n13 p9689-9692, 1 May

## **Solid State Physics**

Keywords: \*Superconductors, Electron phonon interactions, Shear modulus, Bulk modulus, Modulus of elasticity, Poisson ratio, Critical temperature, Bismuth oxides, Lead oxides, Strontium oxides, Calcium oxides, Polycrystalline, Reprints, \*High temperature superconductors, Young modulus, Debye temperature, Kresin model, Temperature dependence, Curvates

For polycrystalline (Bi-Pb)2Sr2Ca2Cu3O10, the authors report the 5-295-K elastic constants: shear modulus (G), Young modulus (E), bulk modulus (B), and Poisson ratio (nu). Both G and E show nearly normal temperature variation. During cooling, B softens between 215 and 65 K. The Poisson ratio decreases abruptly at 215 K and decreases almost five percent in the 295-5-K region. In its temperature dependence, this compound resembles YBa2Cu3O7. However, it shows much lower elastic stiffness. Corrected to the void-free state, the authors calculate a Debye temperature of 312 K, versus 436 K for YBa2Cu3O7. The Poisson ration, 0.20, agrees well with that of YBa2Cu3O7, 0.21. The authors use Kresin's model to interrelate Debye temperature, critical temperature, and electron-phonon interaction parameter for four classes of copper-oxide superconductors.

PB91-134478
Not available NTIS
National Inst. of Standards and Technology (NEL),
Boulder, CO. Electromagnetic Technology Div.
Break Junction Tunneling Spectroscopy of SingleCrystal Bismuth-Based High-Temperature Super-

conductors. Final rept. J. Moreland, C. K. Chiang, and L. J. Swartzendruber.

1990, 7p Pub. in Advances in Cryogenic Engineering (Materials) 36, p619-625 1990.

Keywords: Electron tunneling, Energy gap, Single crystals, Reprints, \*High temperature superconductors, \*Superconducting junctions, Bismuth strontium calcium cuprates, Break junctions.

The authors have measured the tunneling spectra of some high temperature superconducting crystal break junctions at 4 K. The samples were thin plates of Bi2SrCa2Cu2O5 compound. The tunneling spectra (conductance versus voltage) were not typical of BCS superconductor tunneling electrodes. The spectra of higher-resistance break-junction settings (R > 1 M ohm) show a tunneling gap on top of a linearly increasing conductance background signal. 'Harmonic' dip features in the spectra of lower resistance break junction settings (R < 1 M ohm) indicated tunneling between multiple particles in the vicinity of the primary (highest resistance) contact of the junction. The dips occurred at about the same current but shifted in voltage when the resistance of the break junction was continuously adjusted to new settings.

101,463

Not available NTIS PB91-134569 Not available NTIS National Inst. of Standards and Technology (NEL), Boulder, CO. Electromagnetic Technology Div Magnetization of Anisotropic Superconducting Grains.

Final rept. R. L. Peterson, 1990, 4p Pub. in Jnl. of Applied Physics 67, n11 p6930-6933, 1

Keywords: \*Type 2 superconductors, \*Superconductors, Magnetic anisotropy, Magnetic hysteresis, Magnetization, Grain size, Single crystals, Reprints, \*High temperature superconductors, Critical current, Bean

A critical-state calculation of the magnetization of hard type-II superconducting grains having anisotropic critical-current densities is given. The analysis shows how the critical-current densities should be deduced from magnetization measurements for various grain morphologies. A universal curve of the magnetization hysteresis versus one of the grain dimensions is presented, showing that the hysteresis does not change linearly with grain size. Applications to single crystals and to bulk materials are made.

101.464

Not available NTIS PB91-134601 National Bureau of Standards (IMSE), Gaithersburg,

Calculation of Energy of Low-Angle Grain Boundaries.

Final rept. Pub. in Philosophical Magazine A-Defects and Mechanical Properties 55, n4 p499-511 1987.

Keywords: \*Grain boundaries, Reprints, Crystal dislocations, Elasticity.

Various techniques for calculating the linear elastic energy of low-angle grain boundaries are reviewed. The dependence of both elastic and inelastic contributions on boundary-plane orientation (n) and axis of rotation (u) is considered in detail. Particular attention is devoted to the treatment of the elastic contribution near the dislocation cores. The differences in elastic near the dislocation cores. The differences in elastic energy between the recent calculations of Rey and Saada (1977) and Bonnet (1981) with the classic calculation of Read and Shockley (1950) are explained by the differing treatments used by these authors for the region near the cores. The elastic energy for low-angle grain boundaries composed of three sets of parallel, equally spaced dislocations is calculated, within an easily understood convention for handling the region the cores, for the first time. The dependence of the total energy, elastic plus core, on (n) and (u) is given.

101,465

Not available NTIS
National Inst. of Standards and Technology (MSEL),
Gaithersburg, MD. Ceramics Div.
Phase Equilibria in the Suction Stability of the 2122 Phase under Conditions of Oxygen Annealing. Final rept.

L. P. Cook, C. K. Chiang, W. Wong-Ng, L. J. Swartzendruber, and L. H. Bennett. 1990, 4p Pub. in Materials Research Society Symposia Proceedings, v169 p137-140 1990.

Keywords: \*High temperature superconductors, \*Su-perconductors, X-ray diffraction, Magnetic susceptibili-ty, Reprints, \*Thallium barium calcium cuprates, Phase equilibrium.

Results are presented for 850 C oxygen annealing experiments (up to 62 hr) on the 2122 (T1:Ca:Ba:Cu) oxide phase, with and without intermediate grinding. Samples were characterized by powder X-ray diffraction and a.c. magnetic susceptibility. The 2122 phase to be the mendular mirelly, stable in oxygen appears to be thermodynamically stable in oxygen under conditions of both extensive grinding, and, annealing of long duration. However, onset T(c)'s vary from 71 K to 109 K for apparently single-phase 2122 samples with nearly identical X-ray powder patterns, depending upon the heat treatment.

101,466

PB91-147397 Not available NTIS National Bureau of Standards (IMSE), Gaithersburg, MD. Ceramics Div. RIR - Measurement and Use in Quantitative XRD. Final rept. C. R. Hubbard, and R. L. Snyder. 1988, 4p Pub. in Powder Diffraction 3, n2 p74-77 Jun 88.

Keywords: \*X ray diffraction, Quantitative analysis, X ray analysis, Reprints, \*Reference intensity ratio.

The Reference Intensity Ratio (RIR) is a general, instrument-independent constant for use in quantitative phase analysis by the X-ray powder diffraction internal standard method. When the reference standard is co-rundum, RIR is known as I/I(c); These constants are collected in the Powder Diffraction File (1987), can be calculated, and can be measured. Recommended methods for accurate measurement of RIR constants are presented, and methods of using these constants for quantitative analysis are discussed. The numerous, complex constants in Copeland and Bragg's method introduced to account for superimposed lines can be simply expressed in terms of RIR constants and relative intensities. This formalism also permits introduc-tion of constraints and supplemental equations based on elemental analysis.

101.467

Not available NTIS PB91-147603 National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Semiconductor Electronics Div.

Phonon-Assisted Magneto-Donor Optical Transitions in n-InSb.

Final rept. C. L. Littler, W. Zawadzki, M. R. Loloee, X. N. Song, and D. G. Seiler. 1990, 3p Grant NSF-DMR86-17823

Sponsored by National Science Foundation, Washing-

ton, DC. Pub. in Semicond. Sci. Technol. 5, n3S p169-171 Mar

Keywords: \*Indium antimonides, \*Optical transition, Excited states, Phonons, Reprints.

The authors have observed and described new optical transitions between magneto-donor states in InSb as-sisted by optic phonon emission. The phonon-assisted transitions provide a unique opportunity to investigate high excited states of the magneto-Coulomb system. High-resolution data reveal the presence of excited magneto-donor states belonging to the same Landau sub-band.

101,468

PB91-147736 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Semiconductor Electronics Div. Morphology and Barrier-Height Development of Bi/InP(110) Interfaces.

Final rept.
K. E. Miyano, T. Kendelewicz, R. Cao, C. J. Spindt, and I. Lindau. 1990, 7p
Sponsored by Defense Advanced Research Projects Agency, Arlington, VA., and Office of Naval Research,

Arlington, VA. Pub. in Physical Review B 42, n5 p3017-3023, 15 Aug

Keywords: \*Indium phosphides, \*Bismuth, \*Interfaces, Band theory, Substrates, Photoelectron spectroscopy, Reprints.

The development of the interface between cleaved n-and p-type InP(110) substrates and overlayers of Bi has been studied in the coverage range of 0.01 to 10 monolayers with use of soft-x-ray photoemission spec-troscopy. The attenuation and narrowing of the sub-strate in 4d and P 2p core-level spectra, as well as the strate In 4d and P 2p core-level spectra, as well as the line-shape development of the adatom Bi 5d signal, indicate that the morphology is of the Stranski-Krastanov type, as has been verified previously for 5b and Bi over-layers on GaAs(110). Specifically, the Bi grows in ordered two-dimensional patches that merge at 1 monolayer coverage, and beyond the coverage the deposited adatoms form three-dimensional clusters. The band bending as measured from energy shifts of the In 4d and P 2p spectra approaches midgap near 0.3 monolayer coverage, but between 0.3 and 1.0 monolayer the band bending for both doping types exhibits a reversal

101.469

PB91-147926 Not available NTIS National Inst. of Standards and Technology (NEL), Rational first. Or Ordinated and recliniony (NEL), Gaithersburg, MD. Precision Engineering Div. Low Accelerating Voltage SEM Imaging and Me-trology Using Backscattered Electrons. Final rept.

M. T. Postek, 1990, 5p Pub. in Review of Scientific Instruments 61, n12 p3750-3754 Dec 90.

Keywords: \*Scanning electron microscopy, \*Semiconductors, \*Metrology, Microchannel electron multipliers, Electron scattering, Line width, Backscattering, Reprints.

An approach to measure semiconductor structures for nondestructive submicrometer metrology in the scanning electron microscope (SEM) at low accelerating voltage is described, using the collection and meas-urement of only the backscattered electron signal rather than the more commonly used secondary elec-tron signal. In this technique, the backscattered electron signal is collected using a high-efficiency micro-channel-plate electron detector system with the front face of the detector biased negatively to reject the low-energy secondary electrons thus collecting only the backscattered electrons. The advantage of using the backscattered electron signal is discussed, as well as a comparison to measurements using the secondary electron signal. The potential of this technique for application to accurate SEM metrology and standards development is also discussed.

101,470

PB91-148023 Not available NTIS National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Reactor Radiation Div.

Crystal and Spin Structures of Nd2CuO4. Final rept.

S. Skanthakumar, and J. W. Lynn. 1990, 3p Pub. in Physica C 170, p175-177 1990.

Keywords: \*Crystal structure, Single crystals, Tetragonal lattices, Neutron diffraction, X-ray diffraction, Elec-tron spin, Reprints, \*Neodymium cuprates, Magnetic ordering.

X-ray and neutron diffraction have been used to study the magnetic and structural properties of single crystal Nd2CuO4. The authors previously observed a small distortion of the basic tetragonal structure, whereby peaks were observed with both X-ray and neutron dif-fraction. The authors explicity show that these are not due to lambda/2 wavelength contamination, as re-cently suggested. The authors also clarify the nature of the magnetic structures observed in the material. In particular, with the present neutron diffraction data on multidomain samples, it is not possible to distinguish between the collinear and noncollinear spin configurations which have been proposed for this system.

101,471

PB91-148064 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Gas and Particulate Science Div. Secondary Ion Yield Changes in Silicon and Gallium Arsenide Due to Topography Changes during Oxygen or Cesium Ion Bombardment. Final rept.

F. Stevie, P. Kahora, D. Simons, and P. Chi. 1988,

Pub. in Jnl. of Vacuum Science and Technology A 6, n1 p76-80 1988.

Keywords: \*Gallium arsenides, \*Silicon, \*Ion bombardment, Scanning electron microscopy, Oxygen ions, Cesium ions, Topography, Reprints, Secondary ion mass spectroscopy, Depth profiles.

Changes in secondary ion yields of matrix and dopant species have been correlated with changes in surface GaAs. It is concluded that changes in surface topography under O2 ion bombardment can affect secondary ion yields of matrix and dopant species in Si and GaAs. In light of these observations, the practice of normalizing SIMS dopant profiles to a matrix signal must be reexamined.

101,472

Not available NTIS
National Inst. of Standards and Technology (NEL),
Gaithersburg, MD. Semiconductor Electronics Div.
Strontium-Induced Oxygen Defect Structure and
Hole Doping in La2-xSrxCuO4.
Final rept.

rınal rept.
Z. Tan, M. E. Filipkowski, J. I. Budnick, E. K. Heller, D. L. Brewe, B. L. Chamberland, C. E. Bouldin, J. C. Woicik, and D. Shi. 1990, 4p Sponsored by Department of Energy, Washington, DC. Pub. in Physical Review Letters 64, n22 p2715-2718, 28 May 90.

Keywords: \*High temperature superconductors, \*Superconductors, Strontium additions, Crystal defects, Doped materials, Polycrystalline, Reprints, \*Lanthanum strontium cuprates, Lanthanum cuprates.

The authors have discovered that the apical oxygen with a 2.35-A La-O bond length is removed when La is substituted by Sr in polycrystalline La(2-x)Sr(x)CuO4 under normal preparation conditions. This apical oxygen can be partially filled by oxygen annealing. It is reasoned that a defect oxygen is trapped at an interstitial site near the Sr atom. The authors present evidence that this defect oxygen is intrinsic to Sr doping, independent of processing conditions. The authors propose that this defect oxygen serves as a mechanism for hole doping similar to that in the superconducting oxygen-rich La2CuO(4+y).

101.473

PB91-148189 Not available NTIS National Inst. of Standards and Technology (NEL), Boulder, CO. Electromagnetic Technology Div.

Cryogenic Properties of Copper (Wall Chart).

Final rept. C. A. Thompson, W. M. Manganaro, and F. R. Fickett. 1990, 1p

Keywords: \*Copper, \*Copper alloys, \*Graphs(Charts), \*Magnetic properties, \*Electrical resistivity, \*Thermodynamic properties, Cryogenics, Magnetoresistivity.

The document is a wall chart prepared using data selected from the extensive literature on the low temperature properties of copper and from the author's measurements made over the past two decades. It is a successor to, and an update of, an earlier chart with the

101,474 PB91-148205 Not available NTIS National Inst. of Standards and Technology (IMSE), Gaithersburg, MD. Ceramics Div.

Strength and Fracture Behavior of Ba-Y-Cu-O Su-

perconducting Ceramics.

J. S. Wallace, E. R. Fuller, A. S. Raynes, S. W. Freiman, J. E. Blendell, M. L. Balmer, and M. Hill. 1989, 13p

1989, 13p Pub. in Proceedings of International Symposium on High Temperature Superconducting Compounds: Processing and Related Properties, Las Vegas, NV., February 27-28, 1989, p597-609.

Keywords: \*High temperature superconductors, \*Superconductors, Fracture strength, Phase transformations, Microcracks, Toughness, Strains, Reprints, \*Yttrium barium cuprates.

Mechanical reliability is an important aspect of the technological application of high-temperature ceramic superconductors. The paper discusses the strength and fracture behavior of Ba-Y-Cu-O superconducting ceramics, and, more importantly, the influence that the microstructures of these materials impart to the mechanical properties. The sintering conditions are seen to have a profound influence on the microstructure development in these materials. In addition, large internal strains can develop on cooling from the sintering temperature. These strains result either from the phase transformation that occurs during oxygenation or from anisotropy in the thermal expansion. Since strain-relief by plastic deformation or diffusion is generally not active below the sintering temperature in these materials, these strains are most easily accommodated by microcracking. Such microcracking was seen to have a profound influence on the strength behavior.

101,475 PB91-148916 Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Thermophysics Div. Theory of Specific Heat of Solids.

Final rept.

A. P. Miiller, 1988, 89p

Pub. in Specific Heat of Solids, Chapter 1, p1-89 1988.

Keywords: \*Specific heat, Lattice vibrations, Band theory, Superconductors, Spin waves, Spin glass state, Kondo effect, Reviews, Reprints.

A review of the theory describing the contributions of the lattice vibrations, conduction electrons and various magnetic excitations to the specific heat of solids is presented. The lattice contribution is described in terms of a number of models based on the harmonic approximation, namely, the simple Einstein and Debye models and the more realistic Born-von Karman model. The effect of anharmonicity of the lattice vibra-tions and of the formation of lattice vacancies on the specific heat at elevated temperatures is also considered. The contribution of the conduction of the conduction electrons in their normal state is described in terms of the free electron model and deviations from free electron behavior due to band structure and many-body enhancement effects are also discussed. The results for the specific heat of superconducting-The results for the specific heat of superconducting-state electrons as predicted by classical thermody-namics and BCS theory are described. Discussions of theoretical results describing magnetic contributions include the topics: spin-wave specific heat, specific heat in the critical temperature region, Schottky anom-alies and, the Kondo and spin-glass effects. An exten-sive list of references is included.

PB91-148932 Not available NTIS National Inst. of Standards and Technology (NEL), Boulder, CO. Electromagnetic Technology Div.

Possible 'Proximity Matrix' Route to High Current Conductors.

Final rept.

Moreland, Y. Li, J. W. Ekin, and L. F. Goodrich. 1990, 9p

Sponsored by Department of the Navy, Washington,

Pub. in Advances in Cryogenic Engineering (Materials), v36 ptA p413-421 1990.

Keywords: \*High temperature superconductors, \*Superconducting films, \*Yttrium barium cuprates, \*Silver coatings, Electrical conductivity, Vacuum deposition, Proximity effect, Powder(Particles), Reprints.

The conductance of point contacts between the surfaces of superconducting YBa2Cu3O(7-delta) thin films is very low. This is probably due to a native insulating surface layer. The conductance of these point contacts can be markedly increased by vacuum de-positing and subsequently annealing a thin layer of Ag into the surface of the films. The authors believe that what might be described as a normal-metal superconducting 'proximity matrix', is formed at the surface of the Ag coated YBa2Cu3O(7-delta) films. In the paper, they describe their efforts to adapt this method to YBa2Cu3O(7-delta) powder. In particular, they have developed a procedure for vacuum deposition of very thin Ag coatings onto the surface of YBa2Cu3O(X) powder grains. The Ag-treated powder is then pelletized, sintered, annealed, and cut to form small conducting bars for electrical transport testing.

101,477

PB91-149294 Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Quantum Physics Div.

Study of the GaAs-Si(100) Interface Using Laser Probing of Thermal Desorption Kinetics. Final rept.

R. V. Smilgys, D. J. Oostra, and S. R. Leone. 1990,

Contract AFOSR87-0119

Sponsored by Air Force Office of Scientific Research, Bolling AFB, DC.

Pub. in Jnl. of Vacuum Science and Technology B 8, n5 p1102-1108 Sep/Oct 90.

Keywords: \*Gallium arsenides, \*Interfaces, \*Desorption, Laser induced fluorescence, Surface reactions, Silicon, Reprints, Thermal desorption.

The thermal desorption kinetics of Ga from initially Asterminated Si(100) is investigated using laser-induced fluorescence spectroscopy. During the Ga desorption process the surface does not remain fully As terminated because a significant fraction of the initial As coverage simultaneously desorbs with the Ga. The results on the GaAs system are compared with those previously reported on the InAs system, which show that In interacts with As on Si(100) less strongly than does

101,478

PB91-149328 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div. Epitaxial fcc Fe Films on Cu(100).

Final rept.
D. A. Steigerwald, and W. F. Egelhoff. 1988, 1p
Pub. in Physical Review Letters 60, n24 p2558, 13 Jun

Keywords: \*Iron, \*Epitaxial growth, Substrates, Metal films, Magnetic films, FCC lattices, Magnetism, Diffusion, Copper, Reprints.

A comment is given of a recent report on the magnetic properties of ultra-thin films of fcc Fe on Cu(001). The criticism is based on investigations of the epitaxial growth processes in terms of diffusion and segrega-

101.479

PB91-149898 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.

Hall Effect. Final rept.

S. M. Girvin. 1987, 2p See also N87-28431. Pub. in McGraw-Hill Encyclopedia of Science and Technology, p296-297 1987.

## Solid State Physics

Keywords: \*Hall effect, Transport properties, Magnetic fields, Electrical conductivity, Reprints, \*Quantum Hall

The classical and quantum Hall effects are briefly defined and discussed.

101,480

PB91-149963
Not available NTIS
National Inst. of Standards and Technology (NEL),
Boulder, CO. Electromagnetic Technology Div.
Analysis of the YBa2Cu3O7/SrTiO3 Interface as a
Function of Post-Deposition Annealing Temperature.

Final rept.

S. E. Asher, A. J. Nelson, A. R. Mason, A. B. Swartzlander, R. Dhere, L. Kazmerski, J. Halbritter, T. E. Harvey, J. A. Beall, and R. H. Ono. 1990, 7p\_ Pub. in Proceedings of American Vacuum Society Fall Meeting, Boston, Ma., October 10-15, 1990, p205-211.

Keywords: \*High temperature superconductors, \*Superconducting films, \*Yttrium barium cuprates, Strontium titanates, Annealing, Interfaces, Thin films, Re-

A multiple technique approach is used to study YBa2Cu3O7 grown on SrTiO3 as a function of post-deposition annealing temperature. X-ray diffraction data are used to determine the relative amounts of aaxis and c-axis oriented growth. These results are compared to the surface morphology of the films observed by SEM. Secondary ion mass spectrometry (SIMS) is used to study the diffusion of substrate elements into the YBCO films as a function of post-deposition annealing temperature. The data obtained from all these techniques are correlated to determine an optimized temperature for post-deposition annealing. The results of the study show that the desired c-axis oriented growth can be obtained with minimal diffusion of substrate elements into the film at annealing temperatures of 750 C.

101.481 PB91-149997 Not available NTIS National Bureau of Standards (IMSE), Gaithersburg,

Emergence of Modern Nucleation Theory.

Final rept. J. W. Cahn. 1987, 15p Pub. in Materials Research Society Symposia Proceedings, v57 p41-55 1987.

Keywords: \*Nucleation, \*Crystal growth, Theories, Re-

A series of important papers by David Turnbull and his collaborators in the late 1940's and early 1950's laid the experimental and theoretical foundation of modern nucleation theory. The elegance, versatility, and generality of the phenomenological approach, coupled with brilliant and insightful experimental confirmation, sparked widespread application which continues today. Much of David Turnbull's subsequent work in other subjects grew directly or indirectly from that

101,482 PB91-150045 Not available NTIS National Bureau of Standards (IMSE), Gaithersburg, MD. Ceramics Div.

Amorphization and Conductivity of Silicon and Germanium Induced by Indentation.

D. R. Clarke, C. M. Kroll, P. D. Kirchner, R. F. Cook, and B. J. Hockey. 1988, 4p Pub. in Physical Review Letters 60, n21 p2156-2159,

23 May 88.

Keywords: \*Germanium, \*Silicon, Transmission electron microscopy, Electrical conductivity, Indentation, Reprints, \*Amorphization.

The authors report the observation, by transmission electron microscopy, that single crystal silicon and ger-manium is converted to an amorphous state at room temperature directly under both Vickers and Knoop indentations. The effect is seen for crystal orientations of (brackets: 001), (brackets: 011) and (brackets: 111), and with applied loads between 0.1 N and 0.5 N. They also observe that the materials become electrically conducting under load and that the process is reversible on subsequent unloading and reloading. Furthermore, the transformed phase is found to make ohmic contact to the surrounding, untransformed, semiconductor.

101,483 PB91-158501 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Applied and Computational Mathe-

Micromagnetic Calculations of 180 deg Surface Domain-Wall Magnetization Profiles with Comparison to Measurements.

Final rept.

J. L. Blue, and M. R. Scheinfein. 1990, 3p See also PB91-107557. Sponsored by Office of Naval Research, Arlington, VA. Pub. in Jnl. of Applied Physics 68, n12 p6504-6506, 15

Keywords: \*Domain walls, Scanning electron microscopy, Mathematical models, Ferromagnetism, Magnetization, Permalloys, Comparison, Reprints, Landau-Lifshitz-Gilbert equation, Surface magnetism, Micro-

The authors compare measurements of magnetization profiles across 180 deg surface domain walls in a permalloy ferromagnet with calculations from micro-magnetic models. The models were solved both by re-laxation and by a time-evolution calculation. The measurements were made using scanning electron microscopy with polarization analysis. The authors obtain good agreement without postulating any surface ani-sotropy effect. This is the first successful comparison between experiment and a time-evolution calculation of domain walls.

PB91-158642 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Quantum Metrology Group.
X-ray Interferometry and gamma-ray Wave-

lengths.

Final rept.
R. D. Deslattes, 1988, 16p
Pub. in Art of Measurement: Metrology in Fundamental and Applied Physics, p193-208 1988.

Keywords: \*Interferometry, \*X-rays, X-ray diffraction, Crystal structure, Silicon, Reprints.

The role of x-ray interferometry in linking the visible, xray and gamma-ray domains is briefly reviewed, and several applications are considered. Resolution of the conflict between two optical determinations of Si lattice periods is reported.

101,485 PB91-159020 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Gas and Particulate Science Div. Modeling Electron Beam Interactions in Semiconductors.

Final rept.

D. Newbury. 1989, 40p
Pub. in SEM Microcharacterization of Semiconductors, Chapter 2, p29-68 1989.

Keywords: \*Electron beams, \*Semiconductors, Scanning electron microscopy, Beam interactions, Elastic scattering, Monte Carlo methods, Electron trajectories, Mathematical models, Analytic functions, Inelastic scattering, Reprints.

A quantitative description of electron beam - specimen interactions with solids forms the basis for developing models by which scanning electron microscope images of semiconductor materials and devices can be calculated. Elastic and inelastic scattering processes are considered, including both discrete and continuous energy loss descriptions. These processes can be described by analytic functions, and by considering both elastic and inelastic scattering, simulation of individual electron trajectories by Monte Carlo calculations is possible. Applications to specific problems of interest to semiconductor science and technology are described, including spatial resolution at interfaces, details of contrast in charge collection microscopy (electron beam induced conductivity), and energy deposition in solids.

101,486 PB91-159053 Not available NTIS National Inst. of Standards and Technology (IMSE), Gaithersburg, MD. Ceramics Div.
Chemical Modification of the Orthorhombic Superconductor Ba2YCu3O7-delta.

C. P. Ostertag, F. Beech, and E. R. Fuller. 1988, 10p Pub. in Ceramic Transactions 1, n2 p501-510 1988.

Keywords: \*High temperature superconductors, \*Superconductors, Orthorhombic lattices, Chemical reactions, Modification, Silicon carbides, Acetone, Mullite, Reinforcing materials, Whiskers, Milling, Reprints, \*Yttrium barium cuprates.

The superconducting orthorhombic phase of Ba2YCu3O(7-delta) has been observed to undergo a low-temperature chemical reaction with acetone. when used as a milling medium. The chemically modified powder is non-superconducting. The orthorhom-bic structure and superconductivity can be fully regen-erated by annealing in oxygen at 950 C. The modified powder is unstable against and reactive with potential reinforcing materials, such as silicon carbide and mullite whiskers.

101,487

PB91-159129 Not available NTIS National Bureau of Standards (IMSE), Gaithersburg,

MD. Reactor Radiation Div.

Phonon Density of States of Superconducting YBa2Cu3O7 and the Nonsuperconducting Analog YBa2Cu3O6.

Final rept.

J. J. Rhyne, D. A. Neumann, J. A. Gotaas, F. Beech, L. Toth, S. Lawrence, S. Wolf, M. Osofsky, and D. U. Gubser. 1987, 4p Pub. in Physical Review B 36, n4 p2294-2297, 1 Aug

Keywords: \*High temperature superconductors, \*Superconductors, \*Phonons, Orthorhombic lattices, Neutron scattering, Atomic structure, Reprints, \*Yttrium barium cuprates, Density of states.

Neutron scattering has been used to study the vibrational density of states and the atomic structure of the high temperature superconductor YBa2Cu3O7. oxygen atoms were found to occupy four sites and to form chains along the b axis direction of the orthorhombic Pmmm cell. The density of states shows a strong double peak at about 20 meV and a second major maximum near 70 meV with additional less-intense features present at intermediate energies.

101,488

PB91-159772 PC A05/MF A01 National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Reactor Radiation Div. NIST Reactor: Summary of Activities July 1989 through June 1990.
Technical note.

C. O'Connor, Dec 90, 90p NIST/TN-1285 Also available from Supt. of Docs. as SN003-003-03057-1. See also PB90-169996.

Keywords: \*NBSR reactor, Research reactors, Activation analysis, Cold neutrons, Crystal structure, Neutron diffraction, Neutron radiography, Nondestructive tests, High temperature superconductors, Polymeric films, Isotopes, Molecular dynamics, Magnetic semiconduc-

The report summarizes all those programs which use the NIST reactor. It covers the period for July 1989 through June 1990. The programs range from the use of neutron beams to study the structure and dynamics of materials, through nuclear physics and neutron standards to sample irradiations for activation analysis, isotope production, neutron radiography, and nondestructive evaluation.

PB91-161935 Not available NTIS National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Reactor Radiation Div.

Structural and Magnetic Properties of Er Thin Films and Er/Y Superlattices: Magnetoelastic Effects.

Final rept

J. A. Borchers, M. B. Salamon, R. W. Erwin, J. J. Rhyne, and R. R. Du. 1991, 14p Pub. in Physical Review B 43, n4 p3123-3136, 1 Feb

Keywords: \*Erbium, \*Yttrium, Thin films, Superlattices, Molecular beam epitaxy, Magnetic properties, X ray scattering, Magnetization, Neutron diffraction, Comparison, Interfacial tension, Ferromagnetic materials, Magnetoelastic waves, Strain tests, Reprints.

Crystalline erbium thin films and Er/Y superlattices with varying Er-layer thicknesses have been grown by molecular-beam epitaxy. The magnetic and structural

properties of these samples have been analyzed by x-ray-scattering, bulk magnetization, and neutron-diffraction techniques. From a comparison of the data for the two systems, the importance of interfacial strain relative to artificial modulation in shaping the magnetic behavior has been determined. Though the basic nature of the erbium magnetic order is not qualitatively altered in either the thin films or superlattices, the conical ferromagnetic phase is suppressed in all of the samples considered. The enhanced critical fields exhibit a sustantial dependance on Figures this tasks. hibit a systematic dependence on Er-layer thickness. These effects appear to follow directly from the epitaxial basal-plane strain which is measurable in films over 14,000 A thick. The strain, along with a 'clamping' of the Er thermal expansion to the Y lattice, leads to a reduction of the magnitude of the magnetoelastic energy that drives the ferromagnetic transition. The dependence of the magnetoelastic energy on the epitaxial strain is described by a model which accounts for the elastic coupling of the erbium lattice to the yttrium.

PB91-162172 Not available NTIS
National Inst. of Standards and Technology (NML),
Gaithersburg, MD. Electron and Optical Physics Div.
Uses of Spin-Polarised Electrons in Fundamental
Electron-Atom Collision Processes and the Analysis of Magnetic Microstructures.
Final rept. 101,490 PB91-162172

Sis of Magnetic Microsoft States Final rept.

M. H. Kelley. 1990, 18p
Sponsored by Department of Energy, Washington, DC.
Pub. in Australian Jnl. of Physics 43, p565-582 1990.

Keywords: \*Electron-atom collisions, Electron scattering, Ferromagnetic materials, Magnetic storage, Microstructure, Reprints, \*Electron spin polarization, Secondary electrons, Sodium atoms.

Two experimental programs are discussed which exploit the use of polarized electrons for studies of fundamental processes and physical properties. In one program, collisions between spin-polarized electrons and optically pumped sodium atoms provide a very detailed characterization of the spin-dependent interactions important in low-energy electron-atom collisions. The reportant in low-energy electron-atom collisions. The results of these measurements provide a critical test for the reliability of state-of-the-art electron scattering calculations. In the second program, the spin polarization of secondary electrons ejected by high-energy electron impact is used to determine the magnetic structure of ferromagnetic materials with very high spatial resolution (about 60 nm). The ability to perform such studies with high resolution has been exploited both in studies of the basic magnetic properties of ferromagnetic properties of ferromagnetic properties of ferromagnetic properties. studies of the basic magnetic properties of ferromagnetic materials and in studies of how these basic properties affect the magnetic structure and performance of devices used for magnetic information storage.

101,491 PB91-162305 PB91-162305
National Inst. of Standards and Technology (NML),
Gaithersburg, MD. Electron and Optical Physics Div.
Micromagnetics of Domain Walls at Surfaces.

Microllagine Sold Bollian Walls at Surfaces. Final rept.
M. R. Scheinfein, J. Unguris, J. L. Blue, K. J.
Coakley, and D. T. Pierce. 1991, 28p
Sponsored by Office of Naval Research, Arlington, VA.
Pub. in Physical Review B 43, n4 p3395-3422, 1 Feb

Keywords: \*Domain walls, Scanning electron microscopy, Bloch wall, High resolution, Nickel rich permalloy, Magnetic films, Single crystals, Iron, Reprints, Surface magnetism, Neel wall.

High-spatial-resolution magnetization maps of ferromagnetic surfaces are generated with use of scanning electron microscopy with polarization analysis (SEMPA). The structure of surface Neel walls is measured by SEMPA and compared directly to the results of micromagnetics simulations. The authors find that the surface magnetic properties observed with SEMPA can be modeled using standard micromagnetic theory using only bulk parameters. Surface-domain-wall magusing only bulk parameters. Surface-domain-wall magnetization profiles were measured, using two different probe diameters in each case, for an Fe(100) single crystal and for Permalloy films with thicknesses of 0.12, 0.16, 0.20, and 0.24 micrometer. The micromagnetic simulations show the 180 deg wall of the bulk turning over into a Neel wall at the surface with the magnetization in the plane of the surface. The Neel wall extends from the surface into the bulk over a depth approximately equal to a Bloch-wall width.

101,492 PB91-162313

Not available NTIS

National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Semiconductor Electronics Div. Narrow-Gap Semiconductors and Related Materi-Final rept.

D. G. Seiler, and C. L. Littler. 1990, 345p See also AD-A223 534.

Pub. in Jnl. of Semiconductor Science and Technology 5, n5 pS1-S345 May 90.

Keywords: \*Narrow gap semiconductors, \*Semiconductors, \*Meetings, Reprints.

An introduction to the Conference on Narrow Gap Semiconductors and Related Materials held in Gaithesburg, MD, June 12-15, 1989 is given.

101,493 PB91-174532 Not available NTIS
MD. Radiation Physics Div.
Book Review Polaria. Book Review: Polarized Electrons at Surfaces by

J. Kirschner.

Final rept. R. J. Celotta. 1986, 1p Pub. in Applied Optics 25, n12 p1860, 15 Jun 86.

Keywords: \*Surfaces, Polarization(Spin alignment), Reprints, \*Electron spin polarization, Surface magnetism, Book reviews.

The article reviews the book entitled 'Polarized Electrons at Surfaces' by J. Kirschner.

101,494 PB91-174557 Not available NTIS National Inst. of Standards and Technology (NEL),

Gaithersburg, MD. Robot Systems Div.

Development of a Three-Dimensional Finite Element Program for Large Strain Elastic-Plastic Solids.

Final rept.

J. H. Chiou, J. D. Lee, and A. G. Erdman. 1990, 15p Pub. in Computers and Structures 36, n4 p631-645

Keywords: \*Plastic properties, \*Three dimensional models, \*Computer calculations, Mathematical models, Elastic properties, Plastic deformation, Strain rate, Finite element method, Numerical solution, Reprints.

In recent years the progress in computational mechanics has made it possible to adopt more sophisticated constitutive models for solving complicated plasticity problems. For the formulation of elastic-plastic theory at finite strain, E. H. Lee decomposed the deformation gradient into a product of the elastic and plastic parts instead of assuming that the strain rate is the combination of the elastic and plastic strain rates. A finite ele-ment model has been formulated based on E. H. Lee's theory. Accordingly, a three-dimensional general pur-pose finite element software package has been developed. The simple tension problem and the simple shear problem are solved as examples so that the numerical solutions and the exact analytical solutions can be compared. Finally, a tensile test of a thin-walled aluminum alloy tube is solved and compared with the experimental data. The good agreement between the finite element solution and the experimental data demonstrates the validity and applicability of the proposed numerical model.

101,495 PB91-174698 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.

XPS and Auger Forward Scattering in Epitaxial Films.

Final rept. W. F. Egelhoff. 1987, 1p Pub. in Physics Today, pS-69 Jan 87.

Keywords: \*X ray photoelectron spectroscopy, \*Interfaces, \*Epitaxy, Forward scattering, Auger electrons, Thin films, Copper, Nickel, Reprints.

Very recently, a phenomenon long known in angle-re-solved x-ray photoelectron spectroscopy (XPS) has been reinterpreted. The new interpretation is that XPS peak intensities are enhanced at angles corresponding to axes connecting the photoemitting atom to its immediate neighboring atoms. These enhanced intensities thus identify the bond axes present near the surface. In the paper, examples are presented of the great power of the 'XPS searchlight' effect as a new tool for studying epitaxy and interfaces.

101,496

PB91-175232 Not available NTIS National Inst. of Standards and Technology (MSEL),

Gaithersburg, MD. Reactor Radiation Div.

Models for Oxygen Ordering and Diffusion in
Ba2YCu3Ox and Ba2YCu3-yMyOx (M = Fe, Co, AI, Ga). Final rept.

A. Santoro. 1990, 4p Pub. in Materials Research Society Symposia Proceedings, v169 p185-188 1990.

Keywords: \*High temperature superconductors, Vacancies(Crystal defects), Twinning, Substitutes, \*Superconductors, Reprints, \*Yttrium barium cu-

One of the most important aspects of the structure of Ba2YCu3O(x) is the local arrangement of the oxygen atoms on the basal plane of the unit cell for compositions comprised between x=6.0 and x=7.0 (the 'basal plane' is defined by the copper atoms forming the Cu-O2 chains). The paper discusses, from a geometric point of view, models of vacancy formation and ordering in the pure compound, and possible configu-rations of the oxygen atoms in metal doped materials. These models take into account the existence of twinning in samples of composition 6.5 < or = x < or =7.0, are consistent with the observed movement of the twin walls occurring when the oxygen stoichiometry is varied and explain the symmetry and the composition of the metal doped compounds. As the oxygen atoms plane of the structure, in what follows one needs to consider only the atomic configuration on the plane and one may ignore all the other atoms in the unit cell.

PB91-175323 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.

Book Review: 'Polarized Electrons at Surfaces' by

J. Kirschner.

Final rept.

D. T. Pierce. 1986, 1p Pub. in Jnl. of the Optical Society of America B 3, n7 p1040 Jul 86.

Keywords: \*Surfaces. Magnetic materials. Polarization(Spin alignment), Polarized beams, Reprints, \*Electron spin polarization, Book reviews, Surface magnetism.

The application of electron spin polarization to the study of surfaces is a highly exciting and rapidly growing research area. The monograph gives the author's incisive and up-to-date (as of 1984) view of the field. The book has four main parts: Basic Concepts, Experimental Considerations, Results from Non-Magnetic Crystals, and Results from Magnetic Materials. The book is sufficiently self-contained to provide an intro-duction to the field, for students at the graduate level, for example, as well as to serve as a useful reference

101,498

Not available NTIS PB91-175554 National Inst. of Standards and Technology (NML), Gaithersburg, MD. Surface Science Div.

Ion-Induced Radiation-Enhanced Diffusion of

Silver in Nickel. Final rept.

D. Marton, J. Fine, and G. P. Chambers. 1989, 5p Pub. in Materials Science and Engineering A115, p223-227 1989.

Keywords: \*Silver, Auger electron spectroscopy, Metal films, Thin films, Nickel, Reprints, \*Radiation enhanced diffusion, Multilayers.

Radiation-enhanced diffusion (RED) was observed during the Auger electron spectroscopy sputter depth profiling of multilayered Ag/Ni thin films. Broadening of the thin (4 nm) silver layers occurred during sputter profiling and resulted in silver Auger intensity profiles for each of these five layers which were asymmetric, exhibiting a steep leading edge followed by a more slowly decreasing tail. These findings can be interpreted in terms of interface broadening due to two main factors: (1) surface roughening--symmetric broadening; (2) RED of silver--asymmetric broadening. With the model, it has been possible to separate these factors and to determine the rate of RED.

## Solid State Physics

101,499 PB91-175612 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Surface Science Div. Electron Attenuation Lengths at SiO2/Si Interfaces.

J. A. Yarmoff, S. A. Joyce, E. Cartier, and F. R. McFeely. 1990, 7p Pub. in Jnl. of Electron Spectroscopy and Related Phenomena 52, p221-227 1990.

Keywords: \*Silicon dioxide, \*Electron transport, Electron phonon interactions, Kinetic energy, EV range 1-10, EV range 10-100, Photoemission, Interfaces, Reprints, Attenuation length.

The attenuation length, lambda, was measured as a function of kinetic energy for low energy electrons (8-70 eV) traveling through SiO2 with the use of corelevel soft x-ray photoemission. Two oxides of different thickness were compared, and the extra attenuation resulting from the additional oxide on the thicker sample was used to determine the attenuation length. The curve resulting from an analysis which employs an exponential attenuation model displays a minima at an electron kinetic energy of about 35 eV, which is a result of scattering from the bulk plasmon. Below 35 eV, lambda increases and reaches a local maxima at about 20 eV, at which point lambda begins to decrease again. The decrease in lambda at low electron energies arises in part from electron-phonon scattering. This is confirmed by the shape of the bulk Si 2p photoemission peak observed on the thicker oxide sample, which is distorted by the phonon-induced loss processes.

101,500 PB91-178822 PC A23/MF A03 National Inst. of Standards and Technology, Gaithersburg, MD.

Chemistry of Electronic Ceramic Materials. Final rept.

P. K. Davies, and R. S. Roth. Jan 91, 535p NIST/SP-804

Also available from Supt. of Docs. Prepared in cooperation with Pennsylvania Univ., Philadelphia. Sponsored by National Aeronautics and Space Administration, Washington, DC., Office of Naval Research, Arlington, VA., and Idaho National Engineering Lab., Idaho Falls.

Proceedings of the International Conference on the Chemistry of Electronic Ceramic Materials. Held in Jackson, Wyoming on August 17-22, 1990.

Keywords: \*Meetings, \*Ceramics, \*Superconductors, \*Dielectric materials, Dielectric properties, Surface chemistry, Synthesis(Chemistry), Characterization, Crystal growth, Perovskites, Oxides, Computerized simulation.

Partial Contents: Chemical reaction controlled microstructures and properties of ferroelectric ceramics; Chemistry and properties of temperature compensated microwave dielectrics; Molecular chemistry and the synthesis of precursors to electronic ceramic materials; Polymeric synthesis of perovskite powders and films; Electrodeposition of nanomodulated electronic ceramic thin films; Properties of some mixed uranium oxides; The kinetics and mechanism of the crystalliza-tion of Mg2Al4Si5O18 from MgAl2O4 and SiO2 in the presence of a bismuth oxide flux; Alkaline earth nipresence of a bismuth oxide flux; Alkaline earth nitrides and hydrides; Oxygen diffusion in Y2O3-containing tetragonal zirconia polycrystals (Y-TZP); Microstructures in high temperature superconductors; Calorimetric studies of ceramics; Surface energy barrier
formed by adsorbed oxygen in porous ZnO; A scanning tunneling microscopy study of single crystal ZnO
and TiO2 surfaces; Computer simulation studies of and TiO2 surfaces; Computer simulation studies of electronic ceramics; Molecular dynamics simulations of ion motion in divalent and mixed monovalent-divalent beta'-alumina.

101,501 PB91-187294 Not available NTIS National Bureau of Standards (IMSE), Gaithersburg, MD. 6-D Structural Model for the Icosahedral (AI, SI)-Mn Quasicrystal.

Final rept.
J. W. Cahn, D. Gratias, and B. Mozer. 1988, 9p Pub. in Jnl. of Physics 49, n7 p1225-1233 1988.

Keywords: \*Crystal models, Aluminum manganese alloys, Silicon containing alloys, X-ray diffraction, Reprints, \*Quasicrystals, Icosahedral phase.

A 6-dimensional (6-D) periodic model is proposed for the Al-Mn-Si icosahedral quasiperiodic crystal. The model results from an embedding of the periodic cubic alpha structure in 6-D. In the Janner-Janssen-Bak description, it consists of three concentric spherical shells of respectively Mn, Al and Al aligned in perpendicular space around the lattice nodes and two additional shells of Al around the body centers. The model is shown to match the X-ray powder diffraction data with a satisfactory residual R-factor of 0.128.

PR91-187344 Not available NTIS National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Ceramics Div.
Lead Zirconate-Titanate Thin Films Prepared by
the Laser Ablation Technique.

C. K. Chiang, L. P. Cook, P. K. Schenck, P. S. Brody, and J. M. Benedetto. 1990, 7p Pub. in Proceedings of Materials Research Society Symposium Ferroelectric Thin Films, San Francisco, CA., April 16-20, 1990, v200 p133-139.

Keywords: \*Lead zirconate titanates, \*PZT, Ferroelectric materials, Dielectric properties, Electrical resistivity, Thin films, Reprints, Laser ablation.

Lead zirconate-titanate (PZT) thin films were prepared by the laser ablation technique. The PZT (Zr/Ti=53/47) target was irradiated using a focused q-switched Nd:YAG laser (15 ns, 100 mJ at 1.064 micrometers). The as-deposited films were amorphous as indicated by X-ray powder patterns, but crystallized readily with brief annealing above 650C. The dielectric constant and the resistivity of the crystallized films were studied using a parallel-plate type capacitor structure.

PB91-187351 Not available NTIS National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Ceramics Div. Levitation of Superconducting Composites.

Final rept.
C. K. Chiang, M. Turchinskaya, L. J. Swartzendruber, R. D. Shull, and L. H. Bennett. 1990, 5p Pub. in Proceedings of Advances in Materials Science and Applications of High Temperature Superconductors, Greenbelt, MD., April 2-6, 1990, p181-185.

Keywords: \*High temperature superconductors, \*Superconducting composites, Electrical resistivity, Magnetic susceptibility, Magnetic hysteresis, Flux pinning, Levitation, Reprints, \*Yttrium barium cuprates, \*Cyan-

The inverse levitation of a high temperature superconductor-polymer composite consisting of powdered quench-melt-growth Ba2YCu3O(7-delta) and cyanoacrylate is reported. Magnetic hysteresis loop measure-ments for the composite are compared to those meas-ured for the bulk material prior to powdering. Differences in the flux pining capibility bewteen the two ma-terial forms are small but significant.

PB91-187369 Not available NTIS
National Inst. of Standards and Technology (MSEL),
Gaithersburg, MD. Ceramics Div.
Processing Bi-Pb-Sr-Ca-Cu-O Superconductors

from Amorphous State. Final rept. Final Tepl.
C. K. Chiang, W. Wong-Ng, L. P. Cook, S. W. Freiman, N. M. Hwang, M. Vaudin, M. D. Hill, R. D. Shull, A. J. Shapiro, L. J. Swartzendruber, and L. H. Bennett. 1990, 10p

Pub. in Proceedings of Advances in Materials Science and Applications of High Temperature Superconductors, Greenbelt, MD., April 2-6, 1990, p127-136.

Keywords: "High temperature superconductors, "Superconductors, Magnetic susceptibility, Electrical resistivity, Amorphous state, Crystallization, X-rays, Reprints, "Bismuth strontium calcium cuprates.

The bismuth-based high-T(c) superconductors can be processed via an amorphous Bi-Pb-Sr-Ca-Cu oxide. The amorphous oxides were prepared by melting the constituent powders in an alumina crucible at 1200 C in air, followed by pouring the liquid onto an aluminum plate, and rapidly pressing with a second plate. In the amorphous state, no crystalline phase was identified in the powder X-ray diffraction pattern of the quenched materials. After heat treatment at high temperature, the amorphous materials crystallized into a glass-cecontaining a large fraction

Bi2Sr2Ca2Cu3O(x) phase (T(C)=110K). The processing method, crystallization, and results of dc electrical resistivity and ac magnetic susceptibility measurements are discussed.

PB91-187377 Not available NTIS National Inst. of Standards and Technology (IMSE), Gaithersburg, MD. Reactor Radiation Div.

Magnetic Ordering of Er in Powder and Single
Crystals of ErBa2Cu3O7.

T. W. Clinton, and J. W. Lynn. 1991, 4p Pub. in Physica C 174, p487-490 1991.

Keywords: \*High temperature superconductors, \*Superconductors, Temperature measurement, Powder(Particles), Single crystals, Reprints, \*Erbium barium cuprates, \*Magnetic ordering.

A comment is made on the article '2D and 3D Magnetic Ordering of Er in ErBa2Cu3O(x) (6 = or < x = or < 7), by Maletta, et al. We point out that our originally published Meissner Effect data conclusively shows that our sample is fully superconducting, contrary to their assertion. Secondly, we note that our tempera-ture measurements are done via a standard four-probe resistance measurement, which gives a correct value for the resistance of the calibrated thermometer, while their resistance measurements yield values which are systematically high, thus providing an incorrect temperature scale. Hence their own thermometry is in error rather than ours, contrary to their assertion.

101.506 Not available NTIS PB91-189258 National Inst. of Standards and Technology (NML), Gaithersburg, MD. Surface Science Div.

X-ray Photoelectron Forward Scattering Studies of Surface Segregation in Epitaxial Cu-Ni-Ni(100)

Sandwich Structures.

Final rept. W. F. Egelhoff, 1989, 5p Pub. in Jnl. of Vacuum Science and Technology A 7, n3 p2060-2064 1989.

Keywords: \*Surfaces, Electron scattering, Metal films, Photoelectrons, Separation, Epitaxy, Copper, Nickel, X-rays, Reprints, Multilayers

The forward scattering of the Cu 2p(3/2) core level photoelectrons by overlying Ni lattice atoms which occurs in the photoemission process has been used to follow the segregation of Cu to the surface in epitaxial Ni-Cu-Ni(100) sandwich structures. When 1-monolayer of Cu is covered by 1-2 monolayers (ML) of Ni, surface diffusion processes constitute the mechanism by which the segregation occurs, whereas if 1 ML Cu is covered by 10 ML Ni or more, the segregation involves the usual bulk (vacancy) diffusion mechanism.

Not available NTIS PB91-189506 National Bureau of Standards (IMSE), Gaithersburg,

MD. Metallurgy Div.

Magnetic Hysteresis of High-Temperature
YBa2Cu3Ox-AgO Superconductors: Explanation of Magnetic Suspension.

Final rept. C. Y. Huang, Y. Shapira, E. J. McNiff, P. N. Peters, B. B. Schwartz, M. K. Wu, R. D. Shull, and C. K. Chiang. 1988, 6p Pub. in Modern Physics Letters B 2, n7 p869-874 Aug

Keywords: \*High temperature superconductors, \*Superconducting composites, Magnetic hysteresis, Flux pinning, Magnetization, Levitation, Silver oxides, Reprints, \*Yttrium barium cuprates.

The authors have measured the magnetization M of superconducting YBa2Cu3O(x)-AgO composites with T(c) approximately equal to 92 K as a function of an applied magnetic field H at 77 and 87 K. A very pronounced M-H hysteresis loop occurs even at 87 K, indicating the presence of extremely strong pinning with ters. The results of these measurements, together with a simple model, explain quantitatively why these superconductors could be suspended below a magnet.

101.508 Not available NTIS National Bureau of Standards (IMSE), Gaithersburg, MD. Metallurgy Div.

Superconducting Thin Films of Bi-Sr-Ca-Cu-O Obtained by Laser Ablation Processing. Final rept.

B. F. Kim, J. S. Wallace, L. J. Swartzendruber, J. Bohandy, L. H. Bennett, F. J. Adrian, E. Agostinelli, W. J. Green, K. Moojani, R. D. Shull, and T. E. Phillips. 1988, 3p

Pub. in Applied Physics Letters 53, n4 p321-323 1988.

Keywords: \*High temperature superconductors, \*Superconducting films, Electrical resistivity, Thin films, Reprints, \*Bismuth strontium calcium cuprates, Laser ablation, Microwave absorption.

Thin films of Bi-Sr-Ca-Cu-O, deposited on (100) cubic zirconia by laser ablation from a bulk superconducting target of nominal composition BiSrCaCu2O(x), have been investigated by dc resistance and magnetically modulated microwave absorption measurements. The latter technique reveals important features regarding the phase purity of superconducting samples that are masked in the dc resistance measurements. The su-perconducting behavior of the films, as a function of the substrate temperature during deposition and the post-deposition annealing conditions, is discussed.

101,509 PB91-189647 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Chemical Process Metrology Div. Sputtered Thin Film YBa2Cu3On. Final rept.

Final rept.
K. G. Kreider, J. P. Cline, A. Shapiro, J. L. Pena, A. Rojas, J. A. Azamar, L. Maldonado, and L. Del Castillo. 1988, 8p
Pub. in Proceedings of Topical Conference on High Tc Superconducting Thin Films, Devices and Applications of the American Vacuum Society, Atlanta, GA., September 1988, 853-860. tember 1988, p53-60.

Keywords: \*High temperature superconductors, \*Superconducting films, Temperature dependence, Partial pressure, Stoichiometry, Substrates, Oxygen, Sputtering, Thin films, Reprints, \*Yttrium barium cuprates.

The study was carried out to determine the effect substrate temperature, target to substrate angle, and the partial pressure of oxygen in the sputtering atmosphere on the stoichiometry. Films were deposited by planar magnetic sputtering of stoichiometric 1:2:3 pressed and sintered targets on MgO, ZrO2(Y) and ZrO2 coated Al2O3 substrates. DEX and WDS were used to determine the chemical composition of the thin used to determine the chemical composition of the fining. X-ray diffraction was used to identify the structure after film crystallization at 1175K and oxidation at 800K. The partial pressure of oxygen appears to have the most profound effect on the stoichiometry by lowering the barium content. Negative ion resputtering of the growing film apparently also slows film growth rate. Films deposited on alumina circuitboard with a ZrO2 barrier layer have demonstrated transitions to superconducting behavior at 95K when the stoichiometric ratio is preserved.

101,510

PB91-189654 Not available NTIS National Inst. of Standards and Technology (IMSE), Gaithersburg, MD. Ceramics Div. Dynamical Diffraction Imaging (Topography) with

X-ray Synchrotron Radiation.

Final rept. M. Kuriyama, R. C. Dobbyn, and B. W. Steiner. 1989,

Pub. in Annual Review of Materials Science 19, p183-207 1989.

Keywords: Synchrotron radiation, X-rays, Topography, Electrooptics, Reprints, \*Diffraction imaging.

New materials with enormous practical interest are now being produced in industry by far more sophisticated processing methods than those used a decade ago. The structure of these advanced materials is not in a 'stable' state normally found in nature. Even traditional structural materials used for familiar industrial components are virtually all frozen configurationally from states that are metastable or unstable before freezing. Moreover, some materials contain non-equilibrium atomic level dispersions of impurities and topologically metastable structures. In the areas of electronics and electrooptics, materials have already been made with structural control at the atomic level. The wide use of single crystals and single crystal layers as industrial materials requires precise information on atomic behavior during modern processing, such as Czochralski growth and chemical vapor deposition.

Success with such 'high-tech' materials requires the knowledge of new ways to arrange atoms in order to achieve the desired properties.

PB91-189662 Not available NTIS National Bureau of Standards (IMSE), Gaithersburg,

MD. Ceramics Div.

Streaking Images That Appear Only in the Plane of Diffraction in Undoped GaAs Single Crystals: Diffraction Imaging (Topography) by Monochromatic Synchrotron Radiation.

Final rept. M. Kuriyama, U. Laor, D. Larson, R. C. Dobbyn, M. Brown, and B. Steiner. 1988, 7p See also N88-30437.

Pub. in Physical Review B 38, n17 p2421-2427 1988.

Keywords: Monochromatic radiation, Synchrotron radiation, Gallium arsenides, Single crystals, Topography, Reprints, \*Diffraction imaging.

Streaking images restricted to the direction of the dif-Streaking images restricted to the direction of the direction (scattering) vector have been observed on transmission through undoped GaAs. These disruption images (caused by the reduction of diffraction in the direction of observation) appear both in the forward and in Bragg diffracted directions in monochromatic synchrotron radiation diffraction imaging. This previously unobserved phenomenon can be explained in terms of the effective volume of planar defects or platelets which affects the absorption coefficient in anomalous transmission. Such regions of the crystal look perfect despite the presence of imperfections when the scattering vector is not perpendicular to the normal of the platelets.

101,512 PB91-189670 Not available NTIS National Bureau of Standards (NML), Gaithersburg,

MD. Surface Science Div.
Initial Stages of Degradation of Superconductor
Surfaces: O2, H2O, CO2 and CO Chemisorption on La2-xSrxCuO4.

Final rept.
R. L. Kurtz, T. E. Madey, L. Toth, R. Stockbauer, A. Shih, and D. Mueller. 1988, 4p
Pub. in Physical Review B 37, n13 p7936-7939 1988.

Keywords: \*High temperature superconductors, \*Superconductors, \*Chemisorption, Photoelectron spectroscopy, Ultraviolet spectroscopy, Water vapor, Carbon dioxide, Carbon monoxide, Oxygen, Degradation, Surfaces, Reprints, \*Lanthanum strontium curvators.

The initial stages of degradation of high-T(c) superconductor surfaces by interaction with atmospheric gases have been studied using ultraviolet photoelectron spectroscopy. O2 has little effect, while H2O adsorbs dissociatively with an initial sticking coefficient S(o) 1, and forms a surface hydroxide. CO2 adsorbs forming a carbonate like surface species with an initial sticking. carbonate-like surface species with an initial sticking coefficient of 0.3. CO is observed to result in similar adsorbed surface species with a much lower sticking coefficient of 0.0003.

101,513 PB91-189688 PB91-189688 Not available NTIS
National Inst. of Standards and Technology (NML),
Gaithersburg, MD. Surface Science Div.
Electronic Structure of High-Tc Superconductors
Studied Using Photoelectron Spectroscopy.
Final rept. Final rept.

R. L. Kurtz, S. W. Robey, R. L. Stockbauer, D. Mueller, A. Shih, L. Toth, A. K. Singh, and M. Osofsky. 1989, 5p Pub. in Vacuum 39, n7-8 p611-615 1989.

Keywords: \*High temperature superconductors, \*Electronic structure, \*Superconductors, Photoelectron spectroscopy, Synchrotron radiation, Valence bands, Photoemission, Stoichiometry, Carbon dioxide, Carbon monoxide, Water vapor, Oxygen, Surfaces, Reprints, Lanthanum strontium cuprates, Yttrium barium cuprates, Bismuth strontium calcium cuprates, Thallium barium calcium cuprates barium calcium cuprates.

Fundamental information about the structure of the va-Fundamental information about the structure of the varience band and the chemical valence states of the various constituents of the La-Sr-Cu, Y-Ba-Cu, Bi-Sr-Ca-Cu and Ti-Ca-Ba-Cu oxides have been obtained using photoelectron spectroscopy. These results show that the one-electron theories do not adequately describe the electronic structure of these superconductors. The atomic origins of the features observed in the valence bands have been investigated by studying photoemission resonances and changes in excitation cross-sections with photon energy. Results to date suggest that these materials have varying densities of states at the Fermi level, valence bands composed of O 2p and Cu 3d states, and display no significant changes in the band structure associated with the superconducting behavior when the temperature is lowered below T(c). In addition, the complex surface chemistry of these oxides make it essential to study the surface stoichiometry and the interaction of simple molecules. O2 and CO are found to interact only weakly with the surfaces of the materials studied to date, while H2O and CO2 react strongly, forming hydroxides and carbon-

101.514

PB91-189787 Not available NTIS National Inst. of Standards and Technology (IMSE), Gaithersburg, MD. Reactor Radiation Div. Phonon Density of States and Superconductivity in Nd1.85Ce0.15CuO4.

Final rept.

J. W. Lynn, I. W. Sumarlin, D. A. Neumann, J. J. Rush, J. L. Peng, and Z. Y. Li. 1991, 4p Pub. in Physical Review Letters 66, n7 p919-922, 18 Feb 91

Keywords: \*High temperature superconductors, \*Superconductors, Neutron scattering, Inelastic scattering, Electron tunneling, Phonons, Reprints, \*Neodymium cerium cuprates, Density of states.

Inelastic-neutron-scattering techniques have been used to measure the generalized phonon density of states in superconducting Nd(1.85)Ce(0.15)CuO4. There is reasonable agreement at low energies between the authors' measurements and recent pointcontact-tunneling density-of-states measurements reported by Huang et al., which suggests that phonons play a major role in pairing in the electron-superconductor systems. The correspondence at higher energies, however, is not particularly good, but probably reflects the difficulty in obtaining quantitative tunneling data.

101,515 PB91-189928

Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Precision Engineering Div. Microchannel-Plate Detection Systems for Low Accelerating Voltage SEM. Final rept. M. T. Postek. 1991, 8p

Pub. in Hitachi Instrument News, p3-10 Feb 91.

Keywords: \*Scanning electron microscopy, \*Microchannel electron multipliers, Secondary emission, Electron scattering, Line width, Reprints.

Microchannel-plate electron detector systems provide microchannel-plate electron detector systems provide a high gain, low noise capability for low-voltage scanning electron microscopy for the collection of both secondary and backscatteed electrons. Coupled with field emission scanning electron microscopes, such as the Hitachi S-800 and the Hitachi S-4000, microchandel nel-plate detector systems enable the investigation of secondary electron induced contrast mechanisms and backscattered electron detection at extremely low accelerating voltages (i.e., below 1.0 keV for an array of new applications in scanning electron microscopy).

101,516 PB91-189969 PB91-189969 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Gas and Particulate Science Div. Fe Implantation in In0.53Ga0.47As/InP. Final rept.

M. V. Rao, D. S. Simons, P. E. Thompson, N. R. Keshavarznia, J. M. Kuo, P. M. Amirtharaj, and T. Y.

Chang. 1989, 5p Pub. in Jnl. of Applied Physics 65, n2 p481-485 1989.

Keywords: \*Ion implantation, \*Iron, Indium phosphides, Annealing, Reprints, \*Gallium indium arsenides, Secondary ion mass spectroscopy, Depth profiles, Photoreflectance.

Single and multiple energy Fe ion implants are per-formed in n-type InGaAs. Rapid thermal and furnace anneals are used to activate the implanted material. Surface Fe accumulation, multiple Fe peaks and deep in-diffusion of Fe are observed in the secondary ion mass spectrometry depth profiles of the implanted material. The crystal lattice perfection of the annealed

101,516

## Solid State Physics

material is evaluated qualitatively by photoreflectance measurements.

PB91-190090 Not available NTIS Not available N11S
National Inst. of Standards and Technology (NML),
Gaithersburg, MD. Electron and Optical Physics Div.
Geometric and Electronic Properties of Cs Structures on III-V (110) Surfaces: From 1D and 2D Insulators to 3D Metals. Final rept.

L. J. Whitman, J. A. Stroscio, R. A. Dragoset, and R. J. Celotta. 1991, 4p Sponsored by Office of Naval Research, Arlington, VA. Pub. in Physical Review Letters 66, n10 p1338-1341, 11 Mar 91.

Keywords: \*Chemisorption, \*Cesium, Scanning tun-neling microscopy, Indium antimonides, Gallium arsen-ides, Superlattices, Adsorption, Surfaces, Reprints.

The authors report the structural and electronic properties of Cs adsorbed on room-temperature GaAs and InSb (110) surfaces as observed with scanning tunneling microscopy. Cs initially forms long one-dimensional (1D) zigzag chains on both surfaces. Additional Cs adsorption on GaAs(110) results in the formation of a 2D overlayer consisting of five-atom Cs polygons arranged in a c(4x4) superlattice. The tunneling gap measured over these insulating structures narrows with the transition from 1D to 2D, with metallic characteristics observed following saturation with a second Cs overlaver.

101,518 PB91-194662 Not available NTIS
National Inst. of Standards and Technology (NEL),
Boulder, CO. Electromagnetic Technology Div.
YBa2Cu3O7-delta/Insulator Multi-Layers for
Crossover Fabrication Crossover Fabrication.

Final rept. J. A. Beall, M. W. Cromar, T. E. Harvey, M. E. Johansson, and R. H. Ono. 1991, 4p Sponsored by Defense Advanced Research Projects

Agency, Arlington, VA.
Pub. in IEEE (Institute of Electrical and Electronics Engineers) Transactions on Magnetics 27, n2 p1596-1599 Mar 91.

Keywords: \*High temperature superconducters, \*Superconducting films, Strontium titanates, Thin films, Substrates, Dielectrics, Crossovers, Reprints, \*Yttrium barium cuprates, Laser ablation, Multilayers.

The development of thin-film dielectrics compatible with the epitaxial growth of YBa2Cu3O(7-delta)(YBCO) is crucial to the fabrication of multi-layer device and circuit structures. The authors have investi-gated the YBCO/SrTiO3(STO) system by fabricating YBCO/STO bilayers and simple YBCO/STO/YBCO crossover structures. The thin films were deposited in crossover structures. The thirl milms were deposited in situ by pulsed laser deposition and analyzed using x-ray diffraction and scanning electron microscopy. The film interfaces were characterized by secondary ion mass spectrometry (SIMS) depth profiling. They have developed photolithographic and wet-etching processes for patterning the crossovers which are compatible with these materials. The crossover structures were characterized by resistance and insulator pinhole density as well as the superconducting properties of the patterned top and bottom YBCO electrodes (critical temperature, T(c) and critical current density, J(c)). Using SrTiO3 as the insulating layer, they have made crossovers with good isolation between layers (>100 Megohm) and high J(c) even in the top electrode (J(c)(76 K) > 100,000 A/cm squared.

101,519 PB91-194704 Not available NTIS National Inst. of Standards and Technology (NEL), Boulder, CO. Electromagnetic Technology Di Anomalous Low-Frequency Butterfly Curves for Subsidiary and Ferromagnetic Resonance Overlap at 3 GHz. Final rept.

R. W. Cross, C. E. Patton, G. Srinivasan, J. G. Booth, and M. Chen. 1991, 5p Contract USAF-F19628-85-0002

Sponsored by Rome Air Development Center, Griffiss AFB, NY.

Pub. in Jnl. of Applied Physics 69, n3 p1569-1573, 1 Feb 91.

Keywords: \*Yttrium iron garnets, Ferromagnetic resonance, Ultrahigh frequency, Spin waves, Line width, Thin films, Damping, Reprints.

Subsidiary absorption butterfly curves of spin-wave instability threshold versus static in-plane field have been obtained for yttrium iron garnet (YIG) thin films at 3 GHz. The butterfly curves have been found to be rather anomalous, typically displaying a pronounced dip and a very low minimum threshold. These anomalous features are attributed to the overlap of the subsidiary absorption field region with ferromagnetic resonance (FMR). First-order instability theory was extended to include the uniform mode response near rended to include the uniform mode response near FMR. The extended theory yields good fits to the data for reasonable values of the YIG FMR linewidths. The theoretical analysis also shows a predicted flip in the azimuthal propagation angle phi(sub k) for the unsta-ble spin waves in the region of FMR overlap. With increasing field, there are predicted discontinuous changes in phi(sub k) from 90 deg. to 0 deg. and back to 90 deg. in the region of FMR.

101,520 PB91-194738 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.

Soft X-ray Absorption and Emission Spectra and the Electronic Structure of Some Exotic Materials.

D. L. Ederer, L. R. Canfield, T. A. Callcott, K. L. Tsang, C. H. Zhang, and E. T. Arakawa. 1988, 5p See also DE89001207.

Pub. in Proceedings of SPIE (Society of Photo-Optical Instrumentation Engineers) - X-ray Vac. Ultraviolet Interact. Data Bases, Calc., Meas., v911 p75-79 1988.

Keywords: \*Electronic structure, High temperature superconductors, Aluminum manganese alloys, X-ray flu-orescence, X-ray spectroscopy, Soft x-rays, Synchrotron radiation, Absorption spectra, Emission spectra, Band theory, Reprints, Lithium aluminides, Quasicrys-

The technique of soft x-ray fluorescence spectroscopy (SXE) is complimentary to that of photoemission spectroscopy (PES). SXE probes the local partial density of states (PDOS), selects dipole allowed symmetries, and is not necessarily surface sensitive. PES on the other hand, averages over the DOS and can be used to measure the dispersion of the energy bands. PES is also very surface sensitive. The authors present measurements on the high T(c) superconductors, the quasi-crystalline phase of AIMn, and the LiAI intermetallic alloy. These measurements provide insight for theoretical modeling. In the case of the high T(c) compound and the intermetallic compound, the measurements are in good agreement with the theory. However, for the quasicrystals, the measurements provide new insights to challenge theory.

101,521 PB91-194753 Not available NTIS National Inst. of Standards and Technology (NEL), Boulder, CO. Electromagnetic Technology Div Current Record in Superconductors.

Final rept. J. W. Ekin, K. Salama, and V. Selvamanickam. 1991,

Sponsored by Office of Naval Research, Arlington, VA. Pub. in Naturé 350, p26, 7 Mar 91.

Keywords: \*High temperature superconductors, \*Critical current, \*Superconductors, Magnetic fields, Reprints, \*Yttrium barium cuprates.

The authors report the first direct demonstration that high transport J(c) can be achieved in bulk melt-grown YBa2Cu3O7 at magnetic fields up to 30 T at liquid nitrogen temperature.

PB91-194779 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Electron and Optical Physics Div. System for the Study of Magnetic Materials and Magnetic Imaging with the Scanning Tunneling Microscope. Final rept.

P. N. First, J. A. Stroscio, D. T. Pierce, R. A. Dragoset, and R. J. Celotta. 1991, 6p Sponsored by Office of Naval Research, Arlington, VA. Pub. in Jnl. of Vacuum Science and Technology B 9, n2 p531-536 Mar/Apr 91.

Keywords: \*Scanning tunneling microscopy, \*Ferromagnetic materials, Magnetic films, Magnetization, Feasibility, Reprints, Electron spin polarization, Sectional Partners ondary electrons.

A report of work in progress to determine the feasibility of imaging the magnetization of ferromagnetic samples with the scanning tunneling microscope (STM) is presented. A vacuum system was designed to test several different proposals as well as to prepare and characterize thin films of magnetic materials by conventional means, including STM. This was begun with an attempt to detect spatially resolved spin-polarization of secondary electrons emitted from the sample when operating the STM in the scanning field emission mode. Results are currently inconclusive, but encouraging. A weak spin-polarization signal has been observed corresponding to one of the in-plane components of magnetization. However, topographic feedth-rough has not been fully eliminated as a possible spurious source of contrast.

101.523

PB91-194860 Not available NTIS National Inst. of Standards and Technology (MSEL), Boulder, CO. Fracture and Deformation Div.

Group and Phase Sound Velocities in an Eu1Ba2Cu3O7 Superconductor and Related Perovskite Oxides.

Final rept.

H. Ledbetter, C. M. Fortunko, and S. Lin. 1990, 5p Pub. in Proceedings of Ultrasonics Symposium, Hono-lulu, Hl., December 4-7, 1990, p1215-1219.

Keywords: \*Acoustic velocity, \*Superconductors, Barium titanates, Strontium titanates, Phase velocity, Group velocity, Ultrasonic radiation, Reprints, \*Europium barium cuprates.

A material's longitudinal sound-wave velocity relates strongly to the electron-lattice interaction, which affects both conductivity and superconductivity. Measuring phase velocity versus frequency, v(omega), reveals dispersion, which may arise from various sources. To measure v(omega) accurately over a large frequency range, the authors used a modified amplitude-spectrum, pulse-echo method. Specifically, they used a buffer rod whose elastic impedance differed substantially from that of the specimen. Also, they used very broadband ultrasonic transducers and a broadband receiver with large dynamic range. They established the validity of their measurement method by measuring BaTiO3 and SrTiO3 polycrystals. They then used the method to measure the longitudinal-wave velocities in an Eu1Ba2Cu3O7 superconductor, both at 295 and 76 K. Against expectation, they found no remarkable dispersion.

101,524

PB91-194894 Not available NTIS National Bureau of Standards (IMSE), Gaithersburg, MD. Reactor Radiation Div.

Long-Range Antiferromagnetic Order of the Cu in Oxygen Deficient RBa2Cu3O6+x.

Final rept.

W. H. Li, J. W. Lynn, H. A. Mook, B. C. Sales, and Z. Fisk, 1988, 4p

Pub. in Physical Review B 37, n16 p9844-9847 1988.

Keywords: \*High temperature superconductors, \*Anti-ferromagnetism, \*Superconductors, Tetragonal lat-tices, Neutron diffraction, Single crystals, Polarized beams, Copper ions, Reprints, \*Yttrium barium cu-prates, \*Neodymium barium cuprates, \*Magnetic or-

The authors have employed polarized and unpolarized neutron diffraction techniques on both powders and single crystals to establish the nature of the magnetic order of the Cu ions in oxygen deficient RBa2Cu3O(6+x)(R=Y,Nd). Magnetic Bragg peaks of the type (h/2,k/2,l) are observed, which yield a magnetic structure in which the Cu spins are coupled antiferromagnetically both in the Cu-O planes as well as along the tetragonal c-axis, with the spin direction in the tetragonal plane. The Neel temperature is very sensitive to the oxygen content, with T(N)(X approx = 0) approx = 500 K, while the spin configuration is independent of x.

101 525

PB91-194902 Not available NTIS National Inst. of Standards and Technology (IMSE), Gaithersburg, MD. Reactor Radiation Div.

Crystal-Field Splittings in the Cubic Heusler Alloys HoPd2Sn and ErPd2Sn.

Final rept.

N. H. Li, J. W. Lynn, H. B. Stanley, T. J. Udovic, R. N. Shelton, and P. Klavins. 1989, 8p Pub. in Physical Review B 39, n7 p4119-4126, 1 Mar

Keywords: \*Crystal field, Time-of-flight method, Neutron scattering, Inelastic scattering, Magnetic mo-ments, Heusler alloys, Reprints, \*Holmium palladium stannides, \*Erbium palladium stannides, Magnetic superconductors.

Neutron inelastic scattering measurements have been taken with triple-axis and time-of-flight techniques to determine the crystal field levels of the rare-earth ions in the cubic Heusler alloys HoPd2Sn and ErPd2Sn. The observed excitations have been identified as crystal field in origin by their dispersionless character as well as by the temperature and wave-vector dependence of the intensities. Analysis of the data shows that the energies and intensities can be understood on the basis of a crystalline electric field with cubic point symmetry, with Lea, Leask, and Wolf parameters of W = 0.0287(4) meV, x = 0.3248(8) for HoPd2Sn, and W = -0.0450(4) meV, x = 0.3022(6) for ErPd2Sn. The crystal field parameters for the other rare-earth elements have also been calculated by scaling to the values determined for HoPd2Sn.

PB91-194977 Not available NTIS National Inst. of Standards and Technology (IMSE), Gaithersburg, MD. Ceramics Div. Studies of Magnetic Flux Penetration in a Chemi-

cally Synthesized Bi(Pb)SrCaCuO Superconduc-

tor. Final rept.

D. Lundy, J. Ritter, L. Swartzendruber, R. Shull, and L. Bennett. 1989, 7p

Pub. in Jnl. of Superconductivity 2, n2 p273-279 Jun

Keywords: \*High temperature superconductors, \*Superconductors, Magnetic measurement, Magnetic hysteresis, Magnetic flux, Flux pinning, Reprints, \*Bismuth lead strontium calcium cuprates.

Magnetic measurements were conducted on a sample of chemically synthesized Bi(1.5)Pb(0.5)Sr(1.5)Ca(1.75)Cu2O(x) using an ac susceptometer and a vibrating sample magnetometer. The sample showed a large fraction of the phase with a superconducting onset temperature of 110K. This high temperature superconducting phase appears to have an extremely narrow hysteresis loop showing a small number of flux pinning sites.

101.527

PB91-195024 Not available NTIS National Inst. of Standards and Technology (CSTL), Gaithersburg, MD. Surface and Microanalysis Science Div.

Ion Bombardment Induced Diffusion: A Case Study on a Sputtered Ag/Ni Layered System.

D. Marton, and J. Fine. 1990, 19p Pub. in Periodica Polytechnica 34, n1-3 p37-55 1990.

Keywords: \*Diffusion, Ion bombardment, Metal films, Separation, Surfaces, Nickel, Silver, Reprints, Multi-

The layered Ag/Ni system has been shown to exhibit surface segregation of Ag when Ag layer buried be-tween two Ni layers is sputter profiled at room temper-ature (J. Fine et al., 1983). While the study was con-cerned with the analysis of radiation induced segregation (RIS), it also demonstrated the role of bombardment enhanced diffusion in the transport of Ag atoms to the surface. The segregation rate was shown to obey first order kinetic equations, and segregation rates for I keV and 4 keV sputtering were determined.

101,528

PB91-195115 Not available NTIS National Bureau of Standards (IMSE), Gaithersburg,

Wigner-Seitz Local-Environment Study of the High Tc Superconductors.

Final rept.

M. Melamud, L. H. Bennett, and R. E. Watson. 1988,

Pub. in Physical Review B 38, n7 p4624-4631 1988.

Keywords: \*High temperature superconductors, \*Chemical bonds, Wigner-Seitz method, Anisotropy, Reprints, Yttrium barium cuprates, Lanthanum cu-

The neighborhood and bonding of atoms in the high Tc superconductors are studied using a Wigner-Seitz-cell construction. Assuming metallic radii for the atoms, it is shown that the Ba, Y., and La atoms have large coordination numbers. A three-dimensional bonding scheme is suggested. The same bonding characteristics result for both the La-Cu-O type (about 40K) and the Y-Ba-Cu-O type (about 90K) superconductors.

ondary electrons.

101,529 PB91-195461 PB91-195461 Not available NTIS National Inst. of Standards and Technology (NEL),

Gaithersburg, MD. Precision Engineering Div.
SEM Imaging and Metrology at Low Accelerating
Voltages Using Backscattered Electrons. M. T. Postek. 1990, 1p
Pub. in Proceedings of Scanning '91, Atlantic City, NJ.,
April 8-12, 1991, pl-21 1990.

Keywords: \*Scanning electron microscopy, \*Semiconductors, Microchannel electron multipliers, Electron scattering, Backscattering, Metrology, Reprints, Sec-

An approach to measure semiconductor structures for nondestructive submicrometer metrology in the scan-ninng electron microscope (SEM) at low accelerating voltage is described, using the collection and meas urement of only the backscattered electron signal rather than the more commonly used secondary electron signal. In the technique, the backscattered electron signal is collected using a high-efficiency microchannel-plate electron detector system with the front face of the detector biased negatively to reject the low-energy secondary electrons thus collecting only the backscattered electrons. The advantage of using the backscattered electron signal is discussed, as well as a comparison to measurements using the secondary electron signal. The potential of the technique for application to accurate SEM metrology and standards development is also discussed.

101,530 PB91-195552 Not available NTIS

Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Chemical Process Metrology Div. Comparison of Amorphous and Quasicrystalline Films of Sputtered Al0.72Mn0.22Si0.06. Final rept.

J. L. Robertson, S. C. Moss, and K. G. Kreider. 1988,

4p Pub. in Physical Review Letters 60, n20 p2062-2065

Keywords: \*Aluminum manganese alloys, Amorphous materials, Metallic glasses, Sputtering, Thin films, Silicides, Comparison, Reprints, \*Quasicrystals.

collected were on A-ray gata were collected on lilms of Al(0.72)Mn(0.22)Si(0.06) sputtered on NaCl at 45. Films showed a typical metallic glass structure factor, S(Q), while at 230 C the structure was quasicrystalline plus Al. A combined broadening function was applied to the normalized and reduced S(Q) for the 230 C film to bring it essentially into coincidence with the amorphous (45 C) S(Q). This involved both a Lorentzian broadening for particle size and a broadening proportional to Q squared associated with phason strain, and leads the authors to conclude that the glass, or amorphous, phase is a defect limit of the quasicrystal.

Not available NTIS
National Inst. of Standards and Technology (IMSE),
Gaithersburg, MD. Ceramics Div.
Inverse Correlation between the

nescence Excited by Electrons and by Visible Light in Chemical-Vapor-Deposited Diamond Films.

Final rept. L. H. Robins, E. N. Farabaugh, A. Feldman, and L. P. Cook. 1991, 6p Pub. in Physical Review B 43, n11 p9102-9107, 15 Apr

Keywords: \*Cathodoluminescence, \*Photoluminescence, Chemical vapor deposition, Raman spectra, Thin films, Reprints, \*Diamond films.

Diamond films grown by filament-assisted or microwave-plasma-assisted chemical-vapor deposition

(CVD) were characterized by photoluminescence (PL), cathodoluminescence (CL), and Raman spectroscopies. The laser-excited PL spectra of these films in and near the carbon Raman region (1100-1800/cm from the 514.5-nm laser line, or 2.18-2.28 eV) are broad and featureless; CL spectra measured within a wider spectral range (1.5-3.5 eV) shows several distinct components. Because of its correlation with the Raman band of sp2-bonded carbon, the visible-laser-excited PL in the carbon Raman region is attributed to sp2-bonded carbon clusters. The spectrally integrated CL intensity is found to vary from specimen to specimen approximately inversely with the intensity of the laser-excited PL. The inverse correlation is especially strong for one component of the CL, a broad band at 2.85 eV. To explain these results, it is proposed that the luminescence centers in these CVD diamond films can be classified into two types with differing excitation and recombination properties. Rate equations are derived for the luminescence kinetics of such a system of two types of recombination centers.

101,532

PB91-195578 Not available NTIS National Bureau of Standards (IMSE), Gaithersburg, MD. Ceramics Div.

Optically Detected Magnetic Resonance Study of Antisite-to-Acceptor and Related Recombination Processes in as-Grown InP-Zn.

Final rept.

L. H. Robins, T. A. Kennedy, and P. C. Taylor. 1988,

Pub. in Physical Review B 38, n18 p3227-3236 1988.

Keywords: \*Indium phosphides, Electron spin resonance, Magnetic resonance, Point defects, Doped materials, Photoluminescence, Zinc, Reprints, Antisites.

The paramagnetic state of the phosphorus-on-indium The paramagnetic state of the phosphorus-on-indium antisite has been observed by optically detected magnetic resonance (ODMR) in as-grown zinc-doped indium phosphide. The antisite resonance is seen both as an enhancing ODMR signal on the antisite-acceptor photoluminescence (PL) at 0.8 eV and as a quenching ODMR signal on the shallow-donor-acceptor PL at 1.37 eV. The dependence of the ODMR on microwave power, microwave modulation frequency, and photoexcitation intensity is examined, and a rate equation model is developed for the important recombination processes. The experimental results suggest that the antisite-acceptor recombination rate is approximately 40,000/s; the antisite electron spins are unthermalized, but recombine with spin-thermalized holes; and the antisite concentration may be greater than 2 x 10 to the 15th power/cc. Two other resonances are also observed, the shallow donor resonance at g=1.217 and an unidentified broad resonance at g=2.0.

101,533

PB91-195586 Not available NTIS National Inst. of Standards and Technology (IMSE), Gaithersburg, MD. Ceramics Div.

Photoluminescence Excitation by Band-Gap Opti-cal Absorption in Chemical Vapor Deposition Diamond Films.

L. H. Robins, P. J. H. Tjossem, K. C. Smyth, P. Y. Barnes, E. N. Farabaugh, and A. Feldman. 1991, 7p Pub. in Jnl. of Applied Physics 69, n6 p3702-3708, 15

Keywords: \*Photoluminescence, Chemical vapor deposition, Laser spectroscopy, Thin films, Excitation, Reprints, \*Diamond films.

Photoluminescence excitation (PLE) spectra at photon been obtained for diamond films grown by the filament-assisted chemical vapor deposition (CVD) method. The PLE intensity was observed to increase abruptly with photon energy above 5.5 eV. This increase coincides with the onset of phonon-emissionassisted interband absorption, which was observed independently by diffuse transmittance measurements. A lower-energy PLE threshold at about 5.25 eV, which coincides approximately with the onset of phonon-absorption-assisted interband absorption, was observed in the spectrum of a gem-quality natural diamond, but not in the spectra of the CVD-grown films. Emission spectra of the luminescence excited by above-bandgap photons have features similar to luminescence spectra of the same specimens excited by 20-keV electrons. The spectrally integrated intensities of the luminescence excited by above-band-gap photons and by electrons were found to vary from specimen to

## Solid State Physics

specimen in a linearly related manner, suggesting that similar recombination processes occur in both cases.

PB91-195594 Not available NTIS National Inst. of Standards and Technology (NEL), Boulder, CO. Electromagnetic Technology Div. Morphology of Silver on YBa2Cu3O7-delta Thin

Final rept. A. Roshko, R. H. Ono, J. A. Beall, J. Moreland, A. J. Nelson, and S. Asher. 1991, 3p

Pub. in IEEE (Institute of Electrical and Electronics Engineers) Transactions on Magnetics 27, n2 p1616-1618 Mar 91.

Keywords: \*High temperature superconductors, \*Superconducting films, Strontium titanates, Magnesium oxides, Thin films, Microstructure, Morphology, Annealing, Substrates, Silver, Reprints, \*Yttrium barium cuprates, Lanthanum aluminates, Laser ablation.

The morphology of silver layers deposited and annealed on laser ablated YBa2Cu3O(7-delta) films has been examined. Silver was found to dewet the YBa2Cu3O(7-delta) (001) surface on annealing in oxygen and nitrogen. This dewetting behavior may be kineticly inhibited by using either thick silver layers or short anneals and low temperatures. Silver layers for the Appendix of the property thick was studied on films do nm to 2.5 micrometers thick were studied on films de-posited on SrTiO3, LaAlO3 and MgO substrates. Anneal times were varied from 6.5 min to 15 hrs at temperatures from 200 to 700 C.

101,535 PB91-195677 Not available NTIS National Bureau of Standards (IMSE), Gaithersburg, MD. Ceramics Div. Parent Structure of the Layered High-Temperature

Superconductors. T. Siegrist, S. M. Zahurak, D. W. Murphy, and R. S.

Roth. 1988, 2p Pub. in Nature 334, n6179 p231-232 1988.

Keywords: \*High temperature superconductors, \*Crystal structure, \*Superconductors, Tetragonal lattices, X ray diffraction, Reprints, \*Calcium strontium cuprates.

Crystals of composition (Ca(0.86)Sr(0.14))CuO2 have been grown and characterized by single crystal X-ray diffraction. The crystals are tetragonal with space group P4/mmm (No. 123), a = 3.8611(2)A, c = 3.1995(2)A, c/a = 0.829, Z = 1. The structure contains planar CuO2 layers separated by Ca (Sr) atoms. The structure is a simple defect perovskite with ordered even by expensive and can be regarded as the next of the contains the cont dered oxygen vacancies and can be regarded as the n = infinity parent of the A2B2Ca(n-1)Cu(n)O(4+2n) (A = Bi, Tl; B = Sr, Ba) superconductors.

PB91-195743
Not available NTIS
National Inst. of Standards and Technology (NEL),
Gaithersburg, MD. Mathematical Analysis Div.
Effect of an Electric Field on the Morphological
Stability of the Crystal-Melt Interface of a Binary
Alloy. 3. Weakly Nonlinear Theory.
Final rept.

Final rept.

A. A. Wheeler, G. B. McFadden, S. R. Coriell, and D. T. J. Hurle. 1990, 11p See also PB90-193541.

Pub. in Jnl. of Crystal Growth 100, n1-2 p78-88 Feb 90.

Keywords: Binary alloys, Crystal growth, Electric fields, Electromigration, Electroepitaxy, Stability, Reprints, \*Crystal-melt interface.

The effect of a constant electric current on the crystalmelt interface morphology during directional solidifica-tion at constant velocity of a binary alloy is considered. A linear temperature field is assumed, and thermoelectric effects and Joule heating are neglected; electromigration and differing electrical conductivities of crystal and melt are taken into account. A two-dimensional weakly nonlinear analysis is carried out to third order in the interface amplitude, resulting in a cubic amplitude equation that describes whether the bifurcation from the planar state is supercritical or subcritical. For wavelengths corresponding to the most dangerous mode of linear theory, the authors calculate the demarcation between supercritical behavior as a function of processing conditions and material parameters. The bifurcation behavior is a sensitive function of the magnitude and direction of the electric current and of the electrical conductivity ratio.

PB91-195750
Not available NTIS
National Inst. of Standards and Technology (NML),
Gaithersburg, MD. Electron and Optical Physics Div.
Scanning Tunneling Microscopy Study of Clean
and Cs-Covered InSb(110).

L. J. Whitman, J. A. Stroscio, R. A. Dragoset, and R. J. Celotta. 1991, 5p

Sponsored by Office of Naval Research, Arlington, VA. Pub. in Jnl. of Vacuum Science and Technology B 9, n2 p770-774 Mar/Apr 91.

Keywords: \*Indium antimonides, Scanning tunneling microscopy, Crystal defects, Surfaces, Coatings, Cesium, Reprints.

Scanning tunneling microscopy has been employed to study clean and Cs-covered InSb(110) surfaces. Atomic-resolution images of both the filled and empty electronic state densities have been obtained. The surface relaxation determined from these images is in good agreement with that predicted by structure calculations. A variety of surface defects have been ob-served, with the most common appearing to be simple Sb vacancies. Adjacent In and Sb vacancies (Schottky defects) have also been observed. The perturbation of the surface surrounding these defects is asymmetrical along (in brackets: 001), as might be expected due to the asymmetry in the surface. Surprisingly, the perturbation is also asymmetrical along (in brackets: 1,-1,0), where symmetry is expected. Cs adsorbed on room-temperature InSb(110) forms one-dimensional zig-zag chains along (in brackets: 1,-1,0), similar to those previously observed on GaAs(110).

PB91-200865 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Mathematical Analysis Div.
Numerical Study of Two-Dimensional Crystal
Growth Forms in the Presence of Anisotropic Growth Kinetics.

Final rept.
L. N. Brush, and R. F. Sekerka. 1989, 23p
Sponsored by Carnegie-Mellon Univ., Pittsburgh, PA.
Pub. in Jnl. of Crystal Growth, p419-441 1989.

Keywords: \*Crystal growth, \*Two-dimensional calcula-tions, \*Anisotropy, \*Kinetics, Single crystals, Rates(Per time), Morphology, Mathematical models, Liquid-solid interfaces, Fourier transformation, Heat flow, Cooling, Surface tension, Stability, Computation, Quasi-steady states.

A model of the free growth of a two-dimensional single crystal of pure material from an undercooled melt is presented. Quasi-steady-state heat flow and anisotropic interfacial properties couple in the model, governing the morphology of the evolving crystal-melt interface. The evolution of an initially slightly perturbed circular crystal as it grows from the linear into the nonlinear regime both in the absence and in the presence of anisotropic interfacial growth kinetics is studied. The calculations show that in the absence of kinetic anisotropy, splitting of the tip of an initial perturbation occurs. For an initial shape consisting of two Fourier components, a resonant growth effect of the high frequency Fourier component occurs for special initial configurations. Furthermore, the overall rate of crystal growth is shown to be only of the heat extracted from the system and is virtually independent of the interface shape; this is a consequence of the quasi-steady state approxima-tion to heat flow. In the presence of anisotropic growth kinetics, tip stabilization may be observed for certain initial conditions. However, a resonant growth effect can still act to destabilize the tip even in the presence of anisotropic interfacial growth kinetics.

101,539 PB91-203117 Not available NTIS National Inst. of Standards and Technology (NEL), Switching in High-Tc Superconductor Current Transport Measurements.

Final rept. L. F. Goodrich, J. Moreland, and A. Roshko. 1991,

Pub. in IEEE (Institute of Electrical and Electronics Engineers) Transactions on Magnetics 27, n2 p1194-1197 Mar 91.

Keywords: \*High temperature superconductors, Electrical measurement, Critical current, Niobium stannides, Reprints, Switching voltages, Yttrium barium cuprates, Niobium titanium, Weak links.

Switching voltages can occur in four-wire current transport measurements of sintered high-T(c) superconductors. These switching voltages are irreversible shifts in the voltage-current characteristic of the superconductor that result in multiple branches. The voltage along these branches can be very nonlinear as a func-tion of current and can be positive or negative in polari-ty relative to the current direction. These voltages can interface with the correct determination of resistivity and critical current density. Experimental data on unaligned sintered Y1Ba2Cu3O(7-delta) which illustrate the complex nature of the voltages and the confusion they can create are presented. Models based on weak links and H(c1) and on other effects, are discussed as are observations on NbTi and Nb3Sn based superconductors.

101,540 PB91-203539 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Surface Science Div. Core Hole Screening for Intermediate Size Metal

Particles. Final rept

J. A. D. Matthew. 1990, 5p Pub. in Solid State Communication 73, n2 p179-183 1990.

Keywords: \*Dielectric properties, \*Molecular relaxation, \*Metal particles, \*Solid state physics, Electrical properties, Binding, Dielectrics, Metals, Particles, Molecular structure, Reprints.

A hierarchy of dielectric sphere models is presented to account for the shift in binding energy with particle size for a core hole at the center of a jellium sphere of radius R. It is shown that the classical final state interaction between the screening charge deficit at the cluster surface and the localized core hole is indeed very important as recently suggested in the literature, so that for a wide range of R the relaxation energy shift is only weakly dependent on metal dielectric proper-ties. The breakdown of the simple classical rule ob-served below R 20au requires further study both theo-retically and under more controlled experimental conditions.

101,541 PB91-203554 Not available NTIS
NATIONAL STANDARD (NEL), Gaithersburg, MD. Semiconductor Electronics Div.

Lattice Relaxation in Silicon Doped with 4d- and 5d-Transition Metals.

Final rept.

S. Mayo, and J. R. Lowney. 1988, 6p Pub. in Jnl. of Applied Physics 64, n9 p4538-4543

Keywords: \*Silicon, Ionization cross sections, Electron transitions, Conduction bands, Valence bands, Doped materials, Photoionization, Silver, Platinum, Gold, Phonons, Reprints, Lattice relaxation.

Photoionization cross-section spectra from deep centers in silicon doped with technologically important 4d-and 5d-transition elements were analyzed by the Ridley and Amato lattice coupling model to determine threshold energy and lattice relaxation parameters corresponding to optically induced transitions involving either band. The average optic phonon energy is 50 meV. Electron transitions to the conduction band from the silver, platinum, and gold acceptor centers have, respectively, threshold energies (in meV) E(To) = 550, 226, and 570. For silver and gold, the Huang-Rhys parameter S could not be determined because of a mixture of both allowed and forbidden transitions; for platinum, S = 0.3. Electron transition data from the donor centers of these elements to the conduction band are not available or insufficient to allow analysis of the threshold region.

Not available NTIS PB91-203596 National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.

Method of FIM-FEEM Specimen Preparation of Su-

perconducting and Other Oxides. Final rept. A. J. Melmed. 1988, 5p Pub. in Jnl. of Physics C6, p67-71 1988.

Keywords: \*Field ion microscopy, \*Ion microscopy, \*Superconductors, Cuprates, Oxides, Reprints, \*Field electron microscopy.

A new method is described for preparation of oxide specimens for field-ion and field-electron emission microscopy.

101,543 PB91-203604 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.

Progress in Fleld Ion Microscopy Imaging of High-Tc Superconducting Oxides.

Final rept. A. J. Melmed, R. D. Shull, and C. K. Chiang. 1988,

Pub. in Jnl. of Physics C6, p459-464 1988.

Keywords: \*High temperature superconductors, \*Field ion microscopy, \*Superconductors, Image analysis, Reprints, Yttrium barium cuprates, Lanthanum strontium cuprates.

Field ion Microscopy (FIM) of many of the new hightransition-temperature superconducting oxides has become routine. The older La-Sr-Cu-O type and the newer R-Ba-Cu-O ('1,2,3') type, with R= Y, Yb, Sm, newer R-Ba-Cu-O (1,2,3') type, with R= Y, Yb, Sm, Gd, Dy, Ho, Er, Pr, Eu or La, consistently image well at low temperature in hydrogen FIM and argon FIM at higher temperatures, and less consistently in neon FIM. The newest Bi-Sr-Ca-Cu-O type and TI-Ba-Ca-Cu-O type can be imaged by hydrogen FIM, but the Bibased specimens thus far have been mechanically weak and phase identification in both types poses a weak and phase identification in both types poses a significant problem. Some details of FIM image interpretation for the '1,2,3' superconductors are addressed in particular, the various degrees of order in the images and the question of identity of the imaging

101,544 PB91-203612 Not available NTIS National Bureau of Standards (NML), Gaithersburg,

MD. Surface Science Div.
Atomic Fingerprint of YBa2Cu3O7-x-Type High-Temperature Superconductors Observed by Field Ion Microscopy.

Final rept. A. J. Melmed, R. D. Shull, C. K. Chiang, and H. A.

Fowler. 1988, 6p Pub. in Materials Science and Engineering 100, pL27-L32 Apr 88.

Keywords: \*High temperature superconductors, \*Crystal defects, \*Superconductors, Field ion microscopy, Grain boundaries, Crystal dislocations, Twinning, Reprints, Yttrium barium cuprates, Ytterbium barium cuprates, Samarium barium cuprates, Gadolinium barium cuprates.

The high-transition-temperature superconducting oxides YBa2Cu3O(7-x), YbBa2Cu3O(7-x), SmBa2Cu3O(7-x) and GdBa2(Cu(0.96)Fe(0.04))3O(7-x) x)(0 < X < 0.05) have been found to exhibit a common, unusual but characteristic field ion microscope image at low temperatures, due to inhomogeneous field evaporation, field ionization or both, resulting in preferentially imaged atoms. The characteristically striated images enable identification of various lattice defects such as dislocations, twin boundaries and grain boundaries

Not available NTIS
National Inst. of Standards and Technology (NEL),
Boulder, CO. Electromagnetic Technology Div.
Prospects for High Temperature Superconductor-Semiconductor Contacts.
Final rept. 101 545

Final rept. J. Moreland, J. W. Ekin, and T. Larson. 1991, 7p Contract DE-Al05-89ER14044

Contract DE-Al05-89EH14044
Sponsored by Department of Energy, Washington, DC.
Pub. in Proceedings of ASM International Electronic
Materials and Processing Congress (3rd), San Francisco, CA., August 20-23, 1990, p195-201

Keywords: \*High temperature superconductors, \*Semiconductor devices, \*Circuit interconnections, \*Electric contacts, \*Superconductors, Gallium arsenides, Silicon, Reprints, Yttrium barium cuprates, Ohmic contacts.

Development of high temperature superconductor -semiconductor contacts with very low contact resistivi-ties is required for microelectronic applications such as circuit interconnects or superconductor - semiconduc-tor - superconductor (S/Semi/S) proximity effect de-vices. Several thin-film depositon methods have been developed for forming very low resistance contacts to

high temperature superconductors. Such a contact could potentially be part of a superconductor - semi-conductor contact that relies on an intervening normal metal, spanning superconductor and semiconductor interfaces. Presently the authors are surveying materials commonly used to make ohmic contacts to Si and GaAs for their compatibility with high-temperature superconductors. Prime material characteristics necessary for potential contact structures are (1) low chemical reactivity of the intervening materials with high-temperature superconductors, (2) limited interdiffusion of multilayer constituents, and (3) stable, low contact resistivity, ohmic I-V characteristics.

101,546 PB91-203653 Not available NTIS Notional Inst. of Standards and Technology (NEL), Boulder, CO. Electromagnetic Technology Div. Tunnellng Stabilized Magnetic Force Microscopy: Prospects for Low Temperature Applications to Superconductors.

Final rept.

7. Moreland, and P. Rice. 1991, 4p Pub. in IEEE (Institute for Electrical and Electronics Engineers) Transactions on Magnetics 27, n2 p1198-1201 Mar 91.

Keywords: \*Images, \*Tunnel effect, Cryogenics, Superconductors, Magnetic forces, Resolution, Superconducting junctions, Superconducting films, Reprints, \*Tunneling stabilized magnetic force microscopy, Magnetic force microscopes, Flux lattice, Bitter patterns, Yttrium barium cuprates.

The authors have recently demonstrated an imaging technique referred to as tunneling stabilized magnetic force microscopy or TSMFM. TSMFM is performed using a scanning tunneling microscope (STM) with a flexible, magnetic, tunneling tip in place of the usual rigid tunneling tip. TSMFM images are therefore comparation of the control of the c binations of topography and the magnetic forces be-tween the tip and the sample. Room temperature TSMFM images of magnetic bit tracks on a hard disk ISMFM images of magnetic bit tracks on a hard disk have 100 nm resolution and are comparable to Bitter patterns made using a ferrofluid. They have built a low temperature STM with the hope of getting TSMFM images of the flux lattice in superconductors. Preliminary TSMFM images of a YBa(2)Cu(3)O(x) (YBCO) film (T(c) - 88 K) in a 50 mT field show that relatively large magnetic forces are acting on the flevible tin large magnetic forces are acting on the flexible tip while scanning at 48 K.

101,547 PB91-203950 Not available NTIS National Inst. of Standards and Technology (NEL), Boulder, CO. Electromagnetic Technology Div.

Properties of YBa2Cu3O7-delta Thin Films Grown on Off-Axis-Cut MgO Substrates.

S. E. Russek, B. Jeanneret, D. A. Rudman, and J. W. Ekin. 1991, 4p
Pub. in IEEE (Institute of Electrical and Electronics En-

gineers) Transactions on Magnetics 27, n2 p931-934 Mar 91.

Keywords: \*High temperature superconductors, \*Superconducting films, Transition temperature, Magnesium oxides, Crystal growth, Thin films, Substrates, Reprints, \*Yttrium barium cuprates, Sputtered films.

A series of YBa2Cu3O(7-delta) films has been reactively sputtered on off-axis-cut MgO substrates. All the films were oriented with the c axis normal to the substrate regardless of substrate orientation, indicating that growth dynamics is a major factor influencing film orientation on non-lattice-matched substrates. As the substrate orientation is moved off the (100) direction the films showed a decrease in transition temperature and showed properties indicative of an increased den-sity of weak links. The films grown on high-angle substrates showed better properties than the films grown on low-angle substrates. Films grown on (110) MgO were as good as films grown on (100) MgO.

101,548 PB91-216747

(Order as PB91-216705, PC A07/MF A01) National Inst. of Standards and Technology, Gaithers-

National Inst. of Standards and Technology, Gallifersburg, MD. High Resolution Synchrotron X-Radiation Diffraction Imaging of Crystals Grown in Microgravity and Closely Related Terrestrial Crystals.

B. Steiner, R. C. Dobbyn, D. Black, H. Burdette, and M. Kuriyama. 1991, 27p
Prepared in cooperation with EG and G Energy Measurements, Inc., Goleta, CA., National Aeronautics and

Space Administration, Hampton, VA. Langley Research Center, Alabama A and M Univ., Huntsville, and GTE Labs., Inc., Waltham, MA.

Included in Jnl. of Research of the National Institute of Standards and Technology, v96 n3 p305-331 May/Jun

Keywords: \*Crystal growth, \*Crystal defects, X ray diffraction, Synchrotron radiation, Czochralski method, Bridgman method, Mercury iodides, Gallium arsenides, Reduced gravity, High resolution, Electrooptics, Lead tin tellurides, Triglycine sulfates.

Irregularities in three crystals (useful in electrooptic detector research) grown in space and in four terrestrial crystals grown under other wise comparable conditions have been observed in high resolution diffraction imaging. The images provide important new clues to the nature and origins of irregularities in each crystal. For two of the materials, mercuric iodide and lead tin telluride, more than one phase (an array of non dif-fracting inclusions) was observed in terrestrial sam-ples; but the formation of these multiple phases appears to have been suppressed in directly comparable crystals grown in microgravity. The terrestrial seed crystal of triglycine sulfate displayed an unexpected layered structure, which propagated during directly comparable space growth. Terrestrial Bridgman regrowth of gallium arsenide revealed a mesoscopic structure substantially different from that of the original Czochralski material. A directly comparable crystal is to be grown shortly in space.

101 549 PB91-236729 Not available NTIS National Inst. of Standards and Technology (EEEL), Gaithersburg, MD. Semiconductor Electronics Div. Testing the Accuracy of Calculated Equilibrium Carrier Concentrations in the Presence of Surface Fleids. Final rept.

J. Geist, J. R. Lowney, C. R. James, and A. M. Robinson, 1991, 7p Pub. in Jnl. of Applied Physics 70, n1 p236-242, 1 Jul

Keywords: \*Carrier density, One-dimensional calcula-

tions, Charge carriers, Mathematical models, Diffusion theory, Iterative methods, Semiconductors, Tests, Re-

Simple analytic expressions for the one-dimensional, majority-carrier concentration in a uniformly doped, semi-infinite semiconductor with a charge-accumulat-ed front surface are derived. These expressions are based on the assumption that the effective intrinsic carrier concentration depends only upon the concentration of the majority dopant. Within the framework of this assumption, the expressions derived here are rig-orously accurate for intrinsic material, and are accurate to well within 100 parts per million (ppm) for doping concentrations above one trillion/cc. The results of calculations of the majority-carrier concentration carried out using these expressions and using a widely available one-dimensional semiconductor device modeling program are compared to illustrate how these expressions are used for testing the accuracy of iterative solutions of the drift-diffusion equations in the presence of surface fields.

101.550 PB91-236968 Not available NTIS National Inst. of Standards and Technology (EEEL), Gaithersburg, MD. Semiconductor Electronics Div. Majority and Minority Electron and Hole Mobilities in Heavily Doped GaAs. Final rept.

J. R. Lowney, and H. S. Bennett. 1991, 9p Pub. in Jnl. of Applied Physics 69, n10 p7102-7110, 15 May 91.

Keywords: \*Gallium arsenides, \*Electron mobility, \*Hole mobility, Minority carriers, Semiconductor doping, Doped materials, Reprints.

The majority electron and minority hole mobilities have been calculated in GaAs for donor densities between 5 x 10 to the 16th power and 1 x 10 to the 19th power cc. Similarly, the majority hole and minority electron mobilities have been calculated for acceptor densities between 5 x 10 to the 16th power and 1 x 10 to the 20th power cc. All the important scattering mechanisms have been included. The ionized impurity and carriercarrier scattering processes have been treated with a phase-shift analysis. These calculations are the first to

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use a phase-shift analysis for minority carriers scattering from majority carriers. The results are in good agreement with experiment, but predict that at high dopant densities minority mobilities should increase with increasing dopant density for a short range of densities. The results are important for device modeling ecause of the need to have values for minority mobilities.

101,551 PB91-237180 PB91-237180 Not available NTIS National Inst. of Standards and Technology (NEL), Boulder, CO. Electromagnetic Technology Div.

Critical-Current Diffraction Patterns of Grain-Boundary Josephson Weak Links.

Final rept.
R. L. Peterson, and J. W. Ekin. 1990, 5p
Pub. in Physical Review B 42, n13 p8014-8018, 1 Nov

Keywords: \*Josephson junctions, \*Critical current, High temperature superconductors, Superconducting junctions, Diffraction patterns, Grain boundaries, Magnetic fields, Reprints, Weak links.

The authors discuss the diffraction patterns and other characteristics of the critical current as a function of magnetic field in grain-boundary Josephson barriers. Diffraction patterns occur not just for SIS junctions but for all types of Josephson links, including SNS junctions, which may be present at grain boundaries in high-T(c) superconductors. The authors discuss the generality of the Airy diffraction pattern, which is ex-pected to characterize grain-boundary barriers in bulk material more accurately than the Fraunhofer pattern. The transport critical-current density in many bulk, granular high-T(c) superconductors has a power-law dependence on very low magnetic fields, characteristic of averaged diffraction patterns, and cannot be fitted by an exponential magnetic-field dependence, which may result from the material properties of the

101,552 PB91-237263 Not available NTIS National Inst. of Standards and Technology (MSEL),

Gaithersburg, MD. Ceramics Div.
Surface Extended-X-ray-Absorption Fine Structure and Scanning Tunneling Microscopy of Si(001)2x1-Sb.

Final rept. M. Richter, J. C. Woicik, J. Nogami, P. Pianetta, K. E. Miyano, A. A. Baski, T. Kendelewicz, C. E. Bouldin, W. E. Spicer, C. F. Quate, and I. Lindau. 1990, 4p Contract N00014-90-J-1001

Sponsored by Office of Naval Research, Arlington, VA. Pub. in Physical Review Letters 65, n27 p3417-3420, 31 Dec 90.

Keywords: \*Silicon, \*Antimony, \*Interfaces, Scanning tunneling microscopy, X ray absorption, Chemical bonds, Surfaces, Dimers, Reprints, Low energy electron diffraction.

extended-x-ray-absorption fine structure (SEXAFS) has been combined with scanning tunneling microscopy (STM) to determine both the local and long-range bonding properties of the Si(001)2x1-Sb interface. Sb L(3) edge SEXAFS shows that Sb dimers occupy a modified bridge site on the Si(001) surface with a Sb-Sb near-neighbor distance of 2.88 + or -0.03 A. Each Sb atom of the dimer is bonded to two Si atoms with a Sb-Si bond length of 2.63 + or - 0.04 A. STM resolves the dimer structure and provides the long-range periodicity of the surface. Low-energy-electron diffraction of vicinal Si(001) shows that the Sb dimer chains run perpendicular to the original Si dimer

101,553 PB91-237271 Not available NTIS National Inst. of Standards and Technology (CAML), Gaithersburg, MD. Applied and Computational Mathematics Div.

Micromagnetic Calculations of 180 deg Surface Domain Walls.

Final rept. M. R. Scheinfein, and J. L. Blue. 1991, 12p

See also PB91-158501.
Pub. in Jnl. of Applied Physics 69, n11 p7740-7751, 1

Keywords: \*Domain walls, Mathematical models, Mi-crostructure, Permalloys, Iron, Reprints, Landau-Lif-shitz-Gilbert equation, Surface magnetism, Micromag-

The authors compare quantitative results from two methods of solving the micromagnetics equations for 180 deg domain walls. The first method solves the Landau-Lifshitz-Gilbert equation by time integration of the stiff differential equations. The second method uses a relaxation scheme to determine the equilibrium domain wall magnetization configuration. They compare results from these calculations for various damping parameters and discretization mesh densities, and also compare their results with domain wall measure-ments made using scanning electron microscopy with polarization analysis. They conclude that equilibrium domain wall microstructure is insensitive to the damp-ing parameter used in the time method of solution for domain walls in magnetically soft iron and Permalloy. For large damping parameters, the approach to equilibrium is the same for the time method and the relax-ation method. Further, they can obtain metastable equilibrium states with both methods.

101,554 PB91-237289 Not available NTIS Not available NITs
National Inst. of Standards and Technology (PL),
Gaithersburg, MD. Electron and Optical Physics Div.
Scanning Electron Microscopy with Polarization
Analysis (SEMPA)-Studies of Domains, Domain
Walls and Magnetic Singularities at Surfaces and in
Thin Films.

Final rept. M. R. Scheinfein, J. Unguris, M. Aeschlimann, D. T. Pierce, and R. J. Celotta. 1991, 7p See also PB91-112672. Sponsored by Office of Naval Research, Arlington, VA. Pub. in Jnl. of Magnetism and Magnetic Materials 93, 110

p109-115 1991

Keywords: \*Magnetic domains, \*Domain walls, Scanning electron microscopy, Magnetic recording, Magnetic films, Thin films, Magnetooptics, Microstructure, Terbium alloys, Cobalt alloys, Iron alloys, Permalloys, Reprints, \*Surface magnetism, Neel walls, SEMPA system, Electron spin polarization, Micromagnetics

Scanning Electron Microscopy with Polarization Analysis (SEMPA) is used to investigate the surface magnetic microstructure of domain walls in thin permalloy films and the domain structure of magneto-optic TbFeCo alloys. Domain wall measurements confirm the results of micromagnetic theory.

101,555 PB91-237420 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div. Structural Study of the Epitaxial Growth of fcc-Fe Films, Sandwiches, and Superlattices on Cu(100).

D. A. Steigerwald, I. Jacob, and W. F. Egelhoff. Pub. in Surface Science 202, n3 p472-492 1988.

Keywords: \*Iron, \*Epitaxial growth, Metal films, Thin films, Superlattices, Agglomeration, FCC lattices, Magnetism, Substrates, Copper, Reprints.

The epitaxial growth of ultrathin films of pseudomorphic fcc-Fe on Cu(100) has been studied with several structure sensitive techniques. It has been found that structure serisive teamiques. It has been found in the growth is not via a Frank-van der Merwe (layer-by-layer) mechanism, as proposed by several others, but rather exhibits Fe agglomeration, and at or slightly above 300 K, Cu surface segregation. This manner of growth is shown to be consistent with the generally recognized parameters which affect thin film growth. Several adsorbed gas species are found to strongly affect the growth process and the resulting film morphology. The conditions for growth of the best quality Fe films, sandwiches, and superlattices on Cu(100) are presented and are contrasted with the conditions which have been used in previous studies.

Not available NTIS PB91-237438 Not available NTS
National Inst. of Standards and Technology (IMSE),
Gaithersburg, MD. Ceramics Div.
Structural Anomalies in Undoped Gallium Arsenide
Observed in High Resolution Diffraction Imaging
with Monochromatic Synchrotron Radiation.

B. Steiner, M. Brown, R. C. Dobbyn, M. Kuriyama, U. Laor, and Larson. 1989, 10p See also N89-11595.

Pub. in Jnl. of Applied Physics 66, n2 p559-568 1989.

Keywords: \*Gallium arsenides, \*Crystal defects, X ray diffraction, Synchrotron radiation, Monochromatic radi-

ation, Grain boundaries, High resolution, Anomalies,

Novel streak-like disruption features restricted to the plane of diffraction have recently been observed in plane of diffraction have recently been observed in synchrotron radiation diffraction from undoped, semi-insulating gallium arsenide crystals. These features were identified as ensembles of very thin platelets (or interfaces) normal to the various 110 directions, and a structural model consisting of antiphase domain boundaries was proposed. The other principal characteristics observed in high resolution monochromatic synchrotron radiation diffraction images are: (quasi)cellular structure, linear low angle subgrain boundaries in 110 directions, and stripes in a 110 direction, as well as systematic differences in the acceptance. boundaries in 110 directions, and stripes in a 110 direction, as well as systematic differences in the acceptance angle for various diffractions. When these detailed structures are considered together, a unifying picture of these features emerges. That is, the presence of ensembles of thin 110 antiphase platelet regions or boundaries is generally consistent not only with the streak-like diffraction features but with all other observations of defects as well. For the forma-tion of such regions, the authors propose two mechanisms, operating in parallel, that appear to be consist-ent with the various defect features observed by a variety of techniques.

101,557

PB91-237453 PB91-237453 Not available NTIS National Inst. of Standards and Technology (CSTL), Gaithersburg, MD. Surface and Microanalysis Science

Theory of Ballistic-Electron-Emission Spectrosco-py of NiSi2/Si(111) Interfaces.

M. D. Stiles, and D. R. Hamann. 1991, 4p Pub. in Physical Review Letters 66, n24 p3179-3182, 17 Jun 91.

Keywords: \*Nickel silicides, \*Silicon, Scanning tunneling microscopy, Electronic structure, Electron transport, Interfaces, Epitaxy, Reprints, Ballistic electron emission microscopy.

The authors discuss theoretical calculations of ballistic-electron-emission-microscopy spectra based in part on a first-principles computation of the transmission across the interfaces. They propose a way of pre-senting experimental data that highlights the transmission process with respect to contributions from the tunneling distribution. They also present a specific ap-plication to A- and B-type NiSi2/Si(III) interfaces, shwing a factor three difference between them at low voltages.

101,558

PB91-237545 Not available NTIS National Bureau of Standards (IMSE), Gaithersburg,

MD. Metallurgy Div.
Mossbauer Study of the Effect of Oxygen Stoichiometry on the High Tc Superconductor
Y1Ba2(Cu0.97Fe0.03)307-x.

Final rept. L. J. Swartzendruber, L. H. Bennett, M. Z. Harford, and M. Rubinstein. 1988, 12p Pub. in Jnl. of Superconductivity 1, n2 p219-230 1988.

Keywords: \*High temperature superconductors, \*Mossbauer effect, \*Superconductors, Room temperature, Doped materials, Stoichiometry, Iron 57, ature, Doped materials, Stoichiometry, Iron 57, Oxygen, Reprints, \*Yttrium barium cuprates, \*Praseodymium barium cuprates, Magnetic ordering.

The Mossbauer effect of oxygen-depleted YBa2Cu3O(7-x) and PrBa2Cu3O(7-x) doped with 3% (57)Fe has been investigated at room temperature. A (57)Fe has been investigated at room temperature. A manifold of quadrupole-split spectra has been found, wjose parameters are in general agreement with those found by other workers. In addition, the Mossbauer spectra show that a fraction of the Fe sites develop magnetic order at room temperature when the oxygen content is reduced. It is demonstrated that the observed asymmetries in the Mossbauer spectra can be the result of a preferential alignment of the platelike crystallites that arises during the normal sample preparation process. The tendency to bond with the oxygen ration process. The tendency to bond with the oxygen atoms is presumed to be responsible for the discrete-ness of the Mossbauer spectra as a function of oxygen depletion.

101.559

PB91-237552

Not available NTIS

National Inst. of Standards and Technology (MSEL),

Gaithersburg, MD. Metallurgy Div.
Low-Field Flux Pinning in Twinned and Detwinned
Single Crystals of YBa2Cu3O7-x.

Final rept.

L. J. Swartzendruber, D. L. Kaiser, F. W. Gayle, L. H. Bennett, and A. Roytburd. 1991, 3p Pub. in Applied Physics Letters 58, n14 p1566-1568, 8

Keywords: \*High temperature superconductors, \*Flux pinning, \*Superconductors, Single crystals, Twinning, pinning, \*Superconductors, Single Reprints, \*Yttrium barium cuprates.

Flux trapping in single crystals of YBa2Cu3O(7-x) before and after twin removal has been measured for vortices parallel and perpendicular to the c axis. The results show clearly that, for low applied magnetic fields, twins contribute significantly to flux pinning over the temperature range 60 to 85 K when the vortices are parallel to the twin boundaries (i.e., parallel to the c

101.560

PB91-240820 PC A04/MF A01 National Inst. of Standards and Technology (NML), Gaithersburg, MD. Surface Science Div.

Technical Activities 1990 Surface Science Division. C. J. Powell. May 91, 57p NISTIR-4643 See also PB90-161985.

Keywords: Surface chemistry, Surface reactions, Superconducting films, High temperature superconductors, Magnetic recording, Magnetic alloys, Ion irradiation, Synchrotron radiation, Standards, Electron transport, Thin films, Magnetooptics, Semiconductors, Adsorption, Interfaces, Bibliographies, \*Surface science, US NIST.

The report summarizes technical activities and accomplishments of the NIST Surface Science Division during Fiscal Year 1990. Overviews are presented of the Division and of its three constituent groups: Surface Dynamical Processes, Thin Films and Interfaces, and Surface Spectroscopies and Standards. These overviews are followed by reports of selected technical accomplishments during the year. A summary is given of Division outputs and interactions that includes lists of publications, talks, committee assignments, seminars (including both Division seminars and Interface Science seminars arranged through the Division), conferences organized, and a standard reference material certified. Finally, lists are given of Division staff and of guest scientists who have worked in the Division during the past year.

101,561

PB92-108877 PC A03/MF A01 National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Reactor Radiation Div. NIST\*LATTICE: A Program to Analyze Lattice Re-

lationships. Spring 1991 Version.

Technical note (Final).
V. L. Karen, and A. D. Mighell. Sep 91, 41p NIST/

Also available from Supt. of Docs. as SN003-003-03106-2. See also PB86-166774.

Keywords: \*Crystal lattices, \*Computer programming, Programming manuals, Crystal symmetry, Fortran, NIST star LATTICE computer program, Matrix inver-

The NIST \* LATTICE program is written in standard FORTRAN and is designed to be used in any analytical laboratory. The software is multifunctional and can be used to analyze various types of lattice relationships. The present version of the program performs several functions including: (1) the determination of symmetry, and the evaluation of experimental error, through Converse-Transformation analysis; (2) the generation of transformation matrices relating any two unit cells; (3) the calculation of the reduced cell of the lattice, and the calculation and reduction of specified derivative supercells and/or subcells; (4) unit cell transformations; and (5) matrix inversions. It is planned to incorporate additional features in forthcoming versions of the program.

101,562

PB92-109008 PC A08/MF A02 National Inst. of Standards and Technology (MSEL), Gaithersburg, MD.

High Resolution Diffraction Imaging of Crystals Grown in Microgravity and Closely Related Terrestrial Crystals.

Technical note (Final).

B. Steiner, R. Dobbyn, D. Black, H. Burdette, M.

B. Steiner, H. Dobbyn, D. Black, H. Burdette, M. Kuriyama, R. Spal, L. van den Berg, A. Fripp, R. Simchick, R. Lal, A. Batra, D. Mattiesen, and B. Ditchek. Aug 91, 165p NIST/TN-1287
Also available from Supt. of Docs. as SN003-003-03092-9. Sponsored by National Aeronautics and Space Administration, Washington, DC. Microgravity Science and Applications Div.

Keywords: \*Mercury iodides, \*Gallium arsenides, \*Crystal growth, \*Crystal structure, \*Reduced gravity, X ray diffraction, Microgravity applications, Hgl2 semi-conductor detectors, Synchrotron radiation, Monochromatic radiation, High resolution, \*Lead tin tellurides, \*Triplycine sulfates Triglycine sulfates.

The paper reports on irregularities found in three crystals grown in space, in four crystals grown entirely on the ground, and compares the two sets. Irregularities have been observed in mercuric iodide, lead tin telluride, triglycine sulfate, and gallium arsenide by high resolution synchrotron x-radiation diffraction imaging. Radiation detectors made from mercuric iodide crystals grown in microgravity have been reported to perform far better than conventional detectors grown from the same material under full gravity. Effort is now underway to reproduce these 'space' crystals, optimize their properties, and extend comparable superiority to other types of material.

101,563 PB92-112333 PC A05/MF A02 National Inst. of Standards and Technology (MSEL), Boulder, CO. Materials Reliability Div. Oxides and Oxide Superconductors: Elastic and

Related Properties.
M. Lei, and H. Ledbetter. Aug 91, 100p NISTIR-3980

Keywords: \*High temperature superconductors, \*Superconductivity, Electron phonon interactions, Elastic properties, Debye temperature, Bulk modulus, Barium titanates, Strontium titanates, \*Yttrium barium cuprates, Kresin model, Born model.

Using both measurements and modeling, the elastic and related properties of some oxides and oxide superconductors were studied. The polycrystal elastic constants were measured using a MHz-frequency pulse-echo method between 295 and 4 K and corrected to the void-free state by using a model for a composite material containing spherical particles. The elastic moduli of the high-T(c) superconductor Y1Ba2Cu3O7 (YBCO) were compared with that of oxides, especially the perovskites BaTiO3 and SrTiO3, oxides, especially the perovskites BaTiO3 and STTiO3, which are crystal-structure building blocks for the YBCO superconductor. The bulk moduli were also calculated using a Born ionic model with two energy terms: electrostatic (Madelung) and ion-core-repulsion. The calculated bulk modulus of YBCO, 98 GPa, agrees well with measurement, 101 GPa. Based on monocrystal measurements combined with analysistheory, elastic stiffnesses C(ij) for orthorhombic YBCO were estimated. The bulk modulus obtained from the estimated C(ij) by the Voigt-Reuss-Hill averaging method agrees with the monocrystal measurement. From the measured polycrystalline elastic constants, the Debye characteristic temperatures were calculated.

101,564 PB92-116565 Not available NTIS National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Reactor Radiation Div.

Theoretical Model for the Tunneling-Gap Anisotropy Observed in Layered Copper-Oxide High-Temperature Superconductors.

R. C. Casella. 1991, 3p Pub. in Solid State Communications 78, n5 p377-379

Keywords: \*High temperature superconductors, \*Superconductors, Band theory, Single crystals, Reprints, \*Bismuth strontium calcium cuprates, Tunneling gap anisotropy.

A two-band model, in which the pair constituents in one band are linked via double intermediate boson (IB) exchange with a third fermion in the other band, is invoked to understand the tunneling-gap anisotropy observed in Bi2Sr2CaCu2O8 single crystals. The coordinates of the two IBs and of the third fermion are integrated out, leading to effective pair correlations. The theory is presently in agreement with the data and subject to further experimental test via more precise measurements. Within the model, present data imply that the IB cut-off omega > 0.3 eV. The observed broad i.r. excitation centered at approximately 3000/ cm is taken as a candidate for the (possibly composite) IB. Experimental implications are discussed in a general context.

101.565

PB92-116631 Not available NTIS National Inst. of Standards and Technology (CSTL), Gaithersburg, MD. Surface and Microanalysis Science

Magnetic Anisotropies in Ultrathin fcc Fe(001) Films Grown on Cu(001) Substrates.

Final rept.

J. F. Cochran, W. B. Muir, J. M. Rudd, B. Heinrich, Z. Celinski, T. T. Le-Tran, W. Schwarzacher, W. Bennett, and W. F. Egelhoff. 1991, 3p Sponsored by Natural Sciences and Engineering Research Council of Canada, Ottawa (Ontario).

Pub. in Jnl. of Applied Physics 69, n8 p5206-5208, 15

Apr 91. Keywords: \*Thin films, \*Magnetic fields, \*Molecular

beam epitaxy, \*Magnons, Monomolecular films, FCC lattices, Copper, Substrates, Anisotropy, Polishing, Surface finishing, Etching, Smoothing, Brillouin effect, Light scattering, Measurement, Ferromagnetic resonance, Reprints, \*Ultrathin films.

Brillouin light scattering and ferromagnetic resonance have been used to measure the magnetic field dependence of the magnon frequency at room temperature for 3 monolayer thick films of fcc Fe(001) grown by means of molecular beam epitaxy on Cu(001) substrates. These films exhibit a strong uniaxial magnetic anisotropy which causes the magnetization to be oriented perpendicular to the film plane in zero applied field. Four specimens were grown on copper substrates prepared using a chemical polishing technique which avoided the use of abrasives; this treatment greatly reduced the density of etch pits on the copper surface. The uniaxial anisotropies found for these specimens were very consistent and comparable to that previously measured for the best film grown on a mechanically polished copper substrate. There is evidence that substrate smoothness is improved, and hence that the uniaxial anisotropy is increased, when the substrate is covered with a few monolayers of epitaxial copper before the iron films are grown.

101.566

PB92-116680 Not available NTIS National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div.

Single-Target Magnetron Sputter-Deposition of High-Tc Superconducting Bi-Sr-Ca-Cu-O Thin Films.

Final rept.

N. G. Dhere, J. P. Goral, A. R. Mason, R. G. Dhere, and R. H. Ono. 1988, 3p

Pub. in Jnl. of Applied Physics 64, n10 p5259-5261, 15 Nov 88.

Keywords: \*High temperature superconductors, \*Superconducting films, Tetragonal lattices, X ray diffraction, Sputtering, Thin films, Reprints, \*Bismuth strontium calcium cuprates.

Single-target RF magnetron sputtering was used to deposit superconducting thin films of Bi-Sr-Ca-Cu-O with a T(co) above 80 K. Varying P(O2) modified the concentrations of Bi, Cu, and O in the films by 10-20%. Higher annealing temperatures, especially with briemelting, favored the formation of the higher T(c) phases. Tetragonal phases (6-K and 75-K T(c)), with a  $3.8097~A,~c \cdot 24.607~A,~and~Bi2Sr2CuO6~composition, and a <math display="inline">=3.812~A,~c=30.66~A,~and~Bi2Sr(2-x)Ca(1+x)Cu2O8~composition,~were~identified; 70-84~K films~contained~large~proportions~of~a~new~tetragonal~phase, with a <math display="inline">=3.81~A,~and~c=55.23~A.$ 

101,567

PB92-116730 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.

## **Solid State Physics**

Interpretation of Field Ion Microscopy (FIM) images of Asymmetrical Specimens of 1,2,3-Type High-Tc Superconductors. Final rept.

H. B. Elswijk, H. A. Fowler, and A. J. Melmed. 1988,

5p Pub. in Jnl. de Physique 49, nC-6 p489-493 1988.

Keywords: \*High temperature superconductors, \*Field ion microscopy, \*Superconductors, Image analysis, Asymmetry, Reprints, Yttrium barium cuprates.

Field Ion Microscopy (FIM) specimens of '1,2,3'-type high-Tc superconducting materials, typically have an asymmetrical shape. This results from the anisotropic properties, which are involved in the preparation techniques. As a consequence of this shape, the magnification and resolution depend on the direction in the FIM image. Assuming that the elliptical poles in published micrographs are due to tip shape, the authors calculate an asymmetry in the magnification as large as a factor of four. Therefore, the current image interpretation is revisited quantitatively, keeping in mind the magnification asymmetry. The strong effect enhances the striped appearance of the images, and has not been fully recognized so far.

101,568 PB92-117316 Not available NTIS National Inst. of Standards and Technology (NEL), Rational mark of Stationard and February (1927), (1927), (2027

perature Dependence of Eg(x,T).
Final rept.
D. G. Seiler, J. R. Lowney, C. L. Littler, and I. T.
Yoon. 1991, 5p
Pub. in Materials Research Society Symposia Pro-

ceedings, v216 p59-63 1991.

Keywords: \*Mercury cadmium tellurides, Temperature dependence, Energy gap, Carrier density, Nonlinear analysis, Reprints, Magnetoabsorption.

Intrinsic carrier concentrations of narrow-gap Hg(1-x)Cd(x)Te alloys (0.17 = or < x = or < 0.30) have been calculated as a function of temperature between 0 and 300 K by using the new nonlinear temperature dependence of the energy gap obtained previously by two-photon magneto-absorption measurements for samples with 0.24 = or < x = or < 0.26. The authors report here experimental values for E(sub g) (x, T) for samples with x = 0.20 and 0.23 obtained by one-photon magneto-absorption measurements. These data confirm the validity of the new E(sub g) (x, T) relations to the confirmation of tionship for these x values. In this range of composition and temperature, the energy gap of mercury cadmium telluride is small, and very accurate values are needed for the gap to obtain reliable values for the intrinsic carrier density. Large percentage differences exist be-tween their new calculations and previous values for n(sub i) at low temperatures. Even at 77 K, differences approaching 10 percent exist, confirming the importance of using the new n(sub i) results for materials and device characterization and a proper understanding of device operation in long-wavelength materials.

101,569 PB92-117340 Not available NTIS National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Reactor Radiation Div.

Antiferromagnetic Order of Cu in Sm2CuO4.

Final rept. S. Skanthakumar, J. W. Lynn, J. L. Peng, and Z. Y.

Li. 1991, 3p Pub. in Jnl. of Applied Physics 69, n8 p4866-4868, 15 Apr 91.

\*Samarium compounds, \*Cuprates. Keywords: Reywords: Samarium compounds, Cuprates, \*Copper ions, Antiferromagnetism, Neutron diffraction, Single crystals, Ceramics, Comparison, Praseodymium compounds, Neodymium compounds, Tetragonal lattices, Neel temperature, Spin waves, Reprints, Samarium cuprate.

Neutron diffraction techniques have been used to study the magnetic order of the Cu ions in a single crystal of Sm2CuO4. The measurements revealed the development of long-range magnetic order of the Cu moments at T(sub N) = 280 + or - 1 K, with a relatively simple antiferromagnetic configuration of spins as found in Nd2CuO4 and Pr2CuO4. However, the spin directions in Sm2CuO4 are rotated by 90 degrees from the spin directions in Nd2CuO4 and Pr2CuO4. The detailed spin structure can be either collinear or noncol-linear, and in these tetragonal systems it is not possible to distinguish between them with the present neutron diffraction data on multidomain samples. Measurements demonstrate that there are no spin reorientations below the Neel temperature, in contrast to the behavior found for Nd2CuO4.

101,570 PB92-117373 Not available NTIS Not available NTISTS
National Inst. of Standards and Technology (NML),
Gaithersburg, MD. Electron and Optical Physics Div.
Kinematic Theory of Ballistic Electron Emission
Spectroscopy of Silicon-Silicide Interfaces.

M. D. Stiles, and D. R. Hamann. 1991, 5p Pub. in Jnl. of Vacuum Science and Technology B 9, n4 p2394-2398 Jul/Aug 91.

Keywords: \*Cobalt silicides, \*Nickel silicides, \*Silicon, \*Interfaces, Electronic structure, Electron transport, Band theory, Epitaxy, Reprints, Ballistic electron emission spectroscopy.

The electronic structure of the materials being measured has a strong effect on the spectroscopy of the interface between them measured by ballistic electron emission microscopy (BEEM). Specific calculations for CoSi2/Si(111) and NiSi2/Si(111) based on the calculated band structures of the materials illustrate some of the observable effects due to band structures, particularly of the overlayer. The BEEM spectra for CoSi2/Si(111) show a delayed onset due to a mismatch of the states near the conduction band mini-mum in the Si. The spectra for NiSi2/Si(111) show structure due to a decrease in the density of states in the NiSi2 at about 1.8 eV above the Fermi level.

PB92-117381 Not available NTIS National Inst. of Standards and Technology (IMSE),

Gaithersburg, MD.
Theory of Orientation Textures Due to Surface
Energy Anisotropies.

Final rept. J. E. Taylor, and J. W. Cahn. 1988, 3p Pub. in Jnl. of Electronic Materials 17, n5 p443-445

Keywords: \*Crystallization, \*Nucleation, \*Surface energy, Epitaxy, Anisotropy, Substrates, Orientation, Liquid-solid interfaces, Free energy, Surfactants, Wetting, Electronics, Texture, Reprints, Wulff construction.

The effect of surface free energy on the orientation of nuclei on a substrate is examined. In general, the orientation of the nuclei is not determined by minimizing the nucleus-substrate interfacial free energy alone: all interfacial anisotropies must be considered. That orientation preferences should result from anisotropies in the substrate-nucleus interfacial free energies is obvious, but it was found that strong orientation effects are present even if the energy is assumed to be independent of the nucleus orientation, provided that the nutrient-nucleus interfacial free energies are anisotropic. Furthermore, varying the magnitude of even an isotropic nucleus-substrate energy will change the orientation of the nuclei. The theory points to some simple rules for prediction of nucleation orientations.

101,572 PB92-117415 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Electron and Optical Physics Div. Observation of Two Different Oscillation Periods in the Exchange Coupling of Fe/Cr/Fe(100).

J. Unguris, R. J. Celotta, and D. T. Pierce. 1991, 4p Pub. in Physical Review Letters 67, n1 p140-143, 1 Jul

Keywords: \*Magnetization, Scanning electron microscopy, Antiferromagnetism, Ferromagnetism, Chromium, Iron, Oscillations, Magnetoresistivity, Reprints.

Oscillations of ferromagnetic to antiferromagnetic ex-Oscillations of ferromagnetic to antiterromagnetic exchange coupling between two Fe layers separated by a Cr spacer of linearly increasing thickness were investigated by imaging the magnetic domains with scanning electron microscopy with polarization analysis. Up to six oscillations in the coupling with a period of 10-12 Cr layers were observed, and, in the case of an extremely well ordered of 2 Cr layers were observed the project of 2 Cr layers were observed. tions with a period of 2 Cr layers were observed.

101.573 PB92-117464

Not available NTIS

National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Reactor Radiation Div.

Low Temperature Magnetization and Magnetic Ex-

citations in Amorphous Fe78B13Si9.

Final rept.
S. C. Yu, J. W. Lynn, J. J. Rhyne, and G. E. Fish.
1991, 5p
Pub. in Jnl. of Magnetism and Magnetic Materials 97,

p286-290 1991.

Keywords: \*Iron alloys, \*Magnetization, Boron containing alloys, Silicon containing alloys, Amorphous materials, Temperature dependence, Dispersion relations, Neutron scattering, Spin waves, Reprints.

The authors have carried out a study of the low-temperature magnetization and spin-wave dispersion in the amorphous metallic ferromagnet Fe(78)B(13)Si(9). The temperature dependence of the magnetization was measured with a vibrating sample magnetometer was measured with a vibrating sample magnetometer and the spin-wave measurements were carried out using inelastic neutron scattering techniques. The magnetization is found to obey the usual law for M(sub s)(T), while the spin waves follow the conventional ferromagnetic dispersion relation for E(sub q). The spin wave stiffness constant D(T) is found to be substantially larger than the value inferred from the magnetization data similar to the behavior observed in other layer. data, similar to the behavior observed in other Invartype materials.

### Structural Mechanics

PB91-132217 PC A09/MF A01 National Inst. of Standards and Technology (MSEL), Boulder, CO. Materials Reliability Div. Study of Static and Dynamic Fracture Using Strain

J. R. Berger, and J. W. Dally. Sep 90, 188p NISTIR-3952

Keywords: \*Strain measurement, \*Fractures(Materials), \*Crack propagation, Cracking(Fracturing), Strain gages, Strain measuring instruments, Pressure vessels, Algorithms, Least squares method, Accuracy, Steels.

The analysis of strain fields surrounding both stationary and propagating cracks is presented. Series expansions of the static and dynamic strain fields are developed. Gage orientation angles are then studied to optimize the strain response. The orientation angles are found to be dependent on gage type and material. Algorithms are developed which use the temporal or spatial strain variations to extract fracture parameters. The accuracy of the parameter determinations is shown to be excellent, and limits are placed on the validity of the developed methods. The methods are then applied to the analysis of a large scale crack arrest test conducted in a pressure vessel steel. The behavior of the crack-tip position with time and the propagation toughness with time, temperature and position are determined. From this information, details of the conditions at crack arrest are extracted. The prop-agation toughness-crack-velocity relation is then con-

101,575

PB91-147033 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Applied and Computational Mathe-

Mechanism for High Strain-Rate Shear Band Formation.

Final rept.

Pub. in Shock Compression of Condensed Matter 1989, p345-348 1990.

Keywords: \*Torsion tests, Mathematical models, Viscoplasticity, Shear properties, Strains, Reprints.

Two numerical simulations of a model of the highstrain-rate torsion test are discussed, one with isothermal temperature boundary conditions, the other with adiabatic boundary conditions. It is shown that a moving boundary of rigid unloading, starting from isothermal ends of the thin-walled tube, caused by heat conduction, is a plausible mechanism for shear band formation during the test.

## Structural Mechanics

101,576 PB91-147256

Not available NTIS National Inst. of Standards and Technology (MSEL), Boulder, CO. Fracture and Deformation Div.

Experimental and Numerical Studies of the J-Inte-

gral for a Surface Flaw.
Final rept.
R. H. Dodds, and D. T. Read. 1990, 21p
Sponsored by David Taylor Research Center, Bethes-Pub. in International Jnl. of Fracture 43, p47-67 1990.

Keywords: \*Fractures(Materials), \*Fracture properties, \*J integral, \*Crack propagation, Displacement, Deformation, Fracture tests, Tensile stress, Strains, Cracking(Fracturing), Surface properties, Reprints.

Applied J-integral values for a surface cracked tensile panel are experimentally evaluated by measuring strain and displacement quantities along an instrumented contour located on the longitudinal symmetry plane. Nonlinear, 3-D, finite-element analyses are employed to obtain corresponding estimates of the contour and area integral contributions to a 3-D J-integral. Finite element results indicate that the area integral contribution is negligibly small on the symmetry plane; the fracture driving force is thus adequately characterized by the experimental contour values. Detailed comparisons of the experimental and numerical results (crack mouth opening displacement, J-values, and strains along the contour) reveal that the one-quarter symmetric, finite element model accurately predicts

the panel response for overall (gauge length) strains approaching 1.6 times the material yield strain, beyond which the observed deformation patterns exhibited globally asymmetric shear bands. PB91-147371 Not available NTIS National Inst. of Standards and Technology (IMSE), Boulder, CO. Fracture and Deformation Div. Stress Intensity Factors by Enriched Mixed Finite

Final rept. P. R. Heyliger, and R. D. Kriz. 1989, 13p

Pub. in International Jnl. for Numerical Methods in Engineering 28, p1461-1473 1989.

Keywords: \*Fracture mechanics, \*Stress intensity factors, Finite element method, Crack initiation, Fracturing, Stresses, Strains, Elastic properties, Linear systems, Approximation, Displacement, Reprints.

An enriched finite element model for linear elastic fracture mechanics is developed for a mixed variational statement. The independent approximations for the displacement and stress components are enriched by adding the near-field analytic expressions for a cracked body to the polynomial approximations of a conventional element. This allows for an accurate representation of the stress and displacement fields near the crack tip and also results in the direct calculation of the appropriate stress intensity factors. The accuracy of the formulation is demonstrated through several numerical examples.

101,578 PB91-149211

Not available NTIS

National Inst. of Standards and Technology (NML), Boulder, CO. Quantum Physics Div. Thermal Noise in Mechanical Experiments.

Final rept. P. R. Saulson. 1990, 9p Pub. in Physical Review D 42, n8 p2437-2445, 15 Oct

Keywords: \*Mechanical oscillators, \*Thermal noise, Gravitational wave detectors, Suspension devices, Pendulums, Anelasticity, Reprints.

The fluctuation-dissipation theorem is applied to the case of low-dissipation mechanical oscillators, wose losses are dominated by processes occurring inside the material of which the oscillators are made. In the common case of losses described by a complex spring constant with a constant imaginary part, the thermal noise displacement power spectrum is steeper by one power of omega than is predicted by a velocity-damping model. The author constructs models for the thermal noise spectra of systems with more than one mode of vibration, and evaluate a model of a specific design of pendulum suspension for the test masses in a gravitational-wave interferometer.

101,579 PB91-149872

Not available NTIS

National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Applied and Computational Mathe-

Mechanism for Shear Band Formation in the High Strain-Rate Torsion Test.

Final rept.

T. J. Burns. 1990, 9p

See also PB89-215370.

Pub. in Transactions of the ASME 57, p836-844 Dec

Keywords: \*Viscoelasticity, \*Torsion tests, \*Shear properties, Thermoelasticity, Mechanical properties, Rheological properties, Elastic properties, Strains, Stresses, Heat transfer, Plastic flow, Mathematical models, Reprints.

A numerical study of a one-dimensional model of the high strain-rate torsion test shows that a moving boundary of rigid unloading, starting from the ends of the thin-walled tubular specimen, is a plausible mechanism for adiabatic shear band formation during the test. Even though the dimensionless thermal diffusivity parameter is very small, the moving boundary is due to heat transfer from the specimen through its ends, which are assumed to be isothermal heat sinks. The mathematical model is based on a physical model of thermoelastic-plastic flow and a phenomenological Arrhenius model for the plastic flow surface. The numerical technique used is the semi-discretization method of lines.

101,580 PB91-174268 Not available NTIS National Inst. of Standards and Technology (IMSE), Boulder, CO. Fracture and Deformation Div.

Determining the Dynamic Stress Intensity Factor with Strain Gages Using a Crack Tip Locating Algorithm.

J. R. Berger, J. W. Dally, and R. J. Sanford. 1990,

Sponsored by National Science Foundation, Washington, DC.

Pub. in Engineering Fracture Mechanics 36, n1 p145-156 1990

Keywords: \*Strain measurement, \*Stress intensity factors, \*Crack initiation, Strain gages, Stress analysis, Algorithms, Strains, High alloy steels, Fracture mechanics, Crack propagation, Stress concentration, Re-

Recent experimental studies have shown that strain gages can be employed to determine either static or dynamic stress intensity factors, with relatively simple experiments. The paper describes an analysis method for determining stress intensity factors associated with a propagating crack. The analysis is based on a three parameter representation of the strain field near the crack tip. An algorithm is developed where triangulation is used to precisely locate the crack tip position. The algorithm also includes an iteration scheme which permits an accurate determination of two key parameters in the series representation of the strain field. The new method of analysis is demonstrated in a dynamic experiment with a high strength 4340 alloy steel.

Not available NTIS PB91-174433 National Inst. of Standards and Technology (IMSE), Boulder, CO. Fracture and Deformation Div. Improved Optical Diffraction Strain Measurement

System. Final rept.

J. R. Berger, and R. D. Kriz. 1989, 7p

Pub. in Proceedings of SEM Spring Conference on Experimental Mechanics, Cambridge, MA., May 29-June 1, 1989, p572-578.

Keywords: \*Strain measurement, \*Diffraction, \*Laser applications, \*Fracture mechanics, Gratings(Spectra), Optical equipment, Image processing, Strain's, Diffraction patterns, Optical measuring instruments, Crack propagation, Reprints.

Improvements on an automated optical post-processor previously developed at NIST Boulder are described. All three components of in-plane strain as well scribed. All the components of in-plants can determined at a maternal point by observing changes in the diffraction pattern from a high frequency grating. The procedure is automated for full field analysis by using digital image processing and a component of the procedure is automated. essing and a computer controlled positioning device. Spatial resolution and strain sensitivity were improved by decreasing the laser beam diameter, using a separate camera for each diffraction peak, and using frame averaging techniques.

101.582

PB91-174599 Not available NTIS National Inst. of Standards and Technology (IMSE), Boulder, CO. Fracture and Deformation Div.
Use of Birefringent Coatings in Fracture Mechan-

ics.

Final rept

J. W. Dally, J. R. Berger, and K. C. Ham. 1989, 8p. Grant NSF-MSM85-13037

Sponsored by National Science Foundation, Washing-

ton, DC.
Pub. in Proceedings of SEM Spring Conference on Experimental Mechanics, Cambridge, MA., May 29-June 1, 1989, p513-520.

Keywords: \*Strain measurement, \*Stress intensity factors, \*Fracture mechanics, \*Birefringent coatings, Birefringence, Optical equipment, Refractivity, J integral, Plastic deformation, Strains, Elastic properties, Reprints.

The equations which describe the response of birefringent strips, patches and arrays of strips to the strains developed in a plane body with a through thickness crack subjected to opening mode loading are described. The strain-optic equations are shown in terms of K(I) for small scale yielding where an elastic analysis is sufficient. The optical response is also shown in terms of J for a power law hardening material where a plastic region has developed and small scale yielding is not valid. Design concepts for very simple optical gages to measure both K(I) and J are introduced.

101,583

PB91-175208 Not available NTIS National Inst. of Standards and Technology (IMSE), Boulder, CO. Fracture and Deformation Div Computerization of a Thermomechanical Processing Research System.

Final rept.

Y. Rosenthal, and Y. W. Cheng. 1989, 31p Pub. in Intelligent Instruments and Computers, p58-88 Mar/Apr 89.

Keywords: \*Data acquisition, \*Mechanical properties, \*Computerized simulation, Mechanical tests, Software(Computers), Stress strain diagrams, Data analysis, Personal computers, High temperature tests, Processing, Reprints.

Software programs for data acquisition and analysis were developed for a personal computer that operates a thermomechanical processing research system. The programs enable data acquisition during mechanical testing at high temperatures, and at constant true strain rates, as well as enabling post-test data analysis. The system is described and results (mechanical properties, engineering and true stress-strain curves, continuous cooling--transformation diagrams) are presented.

101.584

Not available NTIS PB91-175224 National Bureau of Standards (NEL), Gaithersburg, MD. Structures Div.

Extended Abstract: A Finite Element Study of the

Stress and Displacement Fields Produced by Point Impact.

Final rept

M. Sansalone, N. J. Carino, and N. N. Hsu. 1986, 4p. Pub. in Jnl. of Acoustic Emission 5, n1 pS24-S27 Jan-Mar 86.

Keywords: \*Stress waves, \*Wave propagation, \*Finite element method, \*Displacement, Nondestructive tests, Impact tests, Defects, Greens function, Concretes, Plates, Stresses, Reprints, \*Impact-echo tests.

The National Bureau of Standards is working to develop a nondestructive test method for finding flaws within heterogenous materials, such as concrete. The method, which is referred to as the impact-echo method, involves introducing transient stress waves into a test object by mechanical impact (point source) and monitoring reflections of the waves from internal defects and external boundaries using a displacement transducer (point receiver) which is located close to the impact point. The impact-echo test is a simple procedure; however, successful interpretation of recorded surface displacement waveforms requires an understanding of the interaction of transient stress waves with internal defects. To develop a basis for the

#### Structural Mechanics

method, Green's function solutions, finite element solutions, and experimental studies of transient stress wave propagation in solid plates and in plates containing flaws have been carried out. The abstract will discuss some significant findings of the finite element studies.

Not available NTIS PB91-202812 National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Mathematical Analysis Div. Identification of Dynamic Green's Functions in Structural Networks.

Final rept.

A. S. Carasso, and E. Simiu. 1989, 8p Sponsored by Air Force Office of Scientific Research, Bolling AFB, DC., and Directorate of Aerospace Studies, Kirtland AFB, NM.

Pub. in AIAA (American Institute of Aeronautics and Astronautics) Jnl. 27, n4 p492-499 Apr 89.

Keywords: \*Dynamic structural analysis, \*Greens function, Large space structures, Timoshenko beams, Integral equations, Reprints, III posed problems, Deconvolution.

The paper presents the mathematical and computational basis of a method for experimentally identifying the dynamic behavior of linear structural systems. The method consists of exciting the structure with specific pulses and reconstructing the dynamic Green's func-tions by deconvolution of the measured response. The reconstruction procedure involves the solution of an illposed integral equation in the presence of noise. Inverse Gaussian functions, which have mathematical properties that render the deconvolution problem tractable, are used as probing pulses. Two examples are presented for which dynamic Green's functions are reconstructed from synthetic response data: (1) a non-dispersive medium consisting of a mechanical slider with free body motion, and (2), a network that may be representative of a large orbiting structure, with rigidly connected torsional members and Timoshenko beams. It is shown that residual effects of noise that may be detectable in the reconstructed Green's functions, are effectively smoothed out when these functions are used to predict the response to forces such as may be induced by control systems. Finally, an ex-ample is presented of deconvolution implemented in slow motion.

101.586 PB91-236794 Not available NTIS National Inst. of Standards and Technology (IMSE), Gaithersburg, MD. Fracture and Deformation Div. Resonating-Orthotropic-Cube Method for Elastic Constants.

Final rept. P. Heyliger, H. Ledbetter, and M. Austin. 1990, 10p Pub. in Dynamic Elastic Modulus Measurements in Materials, ASTM STP 1045, p100-109 1990.

Keywords: \*Elastic constants, \*Vibration tests, Piezoelectric transducers, Anisotropy, Mechanical properties, Rayleigh-Ritz method, Reprints.

Following studies by Demarest (1969) and by Ohno (1976), the authors describe measurements and analysis that yield, from a single cube-shape specimen, in a single measurement, the complete set of anisotropic elastic-stiffness constants, the C(ij). Experimentally, they place a cubic specimen between two piezoelectric transducers, which excite and detect the cube's macroscopic free-vibration (fundamental-mode) frequencies, up to 10 MHz. From the specimen's shape, size, and mass, and from the measured resonance-freequency spectrum, they analyze for the C(ij) within a given tolerance.

101,587 PB91-237354 Not available NTIS National Inst. of Standards and Technology (NEL),

Gaithersburg, MD. Structures Div.
Impulse Response Functions for Elastic Structures with Rigid Body Degrees of Freedom. Final rept.

E. Simiu, and G. Cook. 1989, 14p Sponsored by Air Force Office of Scientific Research, Bolling AFB, DC.

Pub. in Jnl. of Sound and Vibration 135, p275-288, 8 Dec 89.

Keywords: \*Dynamic response, \*Greens function, \*Degrees of freedom, \*Elastic analysis, Manipulators, Structural analysis, Functions, Fourier transformation,

Many body problem, Robotics, Structural engineering, Reprints.

A procedure based on the theory of generalized functions is developed which allows the calculation of dy-namic Green's functions for discrete and continuous elastic systems with rigid body degrees of freedom. For any given degree of freedom the procedure divides the Fourier transform of the dynamic Green's function into two parts. The first part contains the singularity due to the rigid body degree of freedom. Its time domain counterpart is obtained in closed form. The second part exhibits no singularities, and its time domain counterpart is obtained by numerical integration using a Fast Fourier Transform routine. The procedure is applied to two systems for which closed form solutions are also obtained: a system consisting of two point masses connected by an elastic spring which slide without friction on a horizontal plane, and a nondispersive mechanical slider with elastic deformations due to shear strain. The agreement between the results yielded by the proposed procedure and the closed form solutions is shown to be excellent. The procedure is then used to caluclate the dynamic Green's function for the tip displacement of a dispersive medium consisting of a flexible robot manipulator with the mechanical properties of a Timoshenko beam.

PB92-116573 Not available NTIS National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Polymers Div.

Buckling and Post-Buckling Behavior of Elliptical Plates: Part 1. Analysis.

Final rept.

H. Chai. 1990, 8p See also Part 2, PB92-116581.

Pub. in Jnl. of Applied Mechanics 57, p981-988 Dec

Keywords: \*Structural analysis, \*Composite structures, \*Plates, \*Elliptical configuration, \*Buckling, Calculation methods, Polynomials, Ritz method, Delaminating, Stress analysis, Displacement, Deformation, Loads(Forces), Substrates, Reprints.

A polynomial series expansion for displacements is used in conjunction with the Rayleigh-Ritz energy method to produce buckling and post-buckling stress solutions for an elliptically-shaped surface layer that has been delaminated from the main load-bearing body. Plate deformations are induced by a combined in-plane displacement field applied to the plate boundary and normal pressure. Convergence of the plate so-lution is assessed by systematically increasing the number of displacement terms in the series expansion. The convergence of membrane and bending stresses at the plate boundary was generally slow and nonuniform. The degrees-of-freedom necessary for a satisfactory solution typically increase with increasing com-plexity or magnitude of the plate deformations. By em-ploying as many as 77 displacement terms, practically exact stress solutions are obtained for a wide variety of basic delamination plate problems. The proposed so-lution procedure is highly efficient and economical, and it may be easily extended to other plate geome-tries of loading conditions.

Not available NTIS National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Polymers Div. Buckling and Post-Buckling Behavior of Elliptical Plates. Part 2. Results.

Final rept. H. Chai. 1990, 6p See also Part 1, PB92-116573. Pub. in Jnl. of Applied Mechanics 112, p989-994 Dec

Keywords: \*Composite structures, \*Delaminating, \*Buckling, Elliptical configuration, Stress analysis, Structural analysis, Graphic methods, Substrates, Membrane structures, Bend tests, Loads(Forces), Displacement, Plates, Reprints.

The large-deflection plate solution developed in Part I is used here to study the buckling and post-buckling deformation and stress characteristics of an elliptically-shaped surface layer that has been delaminated from a large material body. The economical, yet accu-rate nature of the solution, together with available graphic routines, has made it possible to present, figuratively, a comprehensive description of the plate behavior. The conditions for a layer-substrate overlap and the variations of membrane and bending stresses along the plate boundary are emphasized. Deformations were induced either by a normal pressure or a biaxial displacement field applied to the plate boundary. The problem variables are plate size and shape, details of load biaxiality, and load level.

101.590 PB92-126622

(Order as PB92-126614, PC A06/MF A02) National Inst. of Standards and Technology, Gaithersburg, MD.

burg, MD.
Summary of the Intercomparison of the Force
Standard Machines of the National Institute of
Standards and Technology, USA, and the Physikalisch-Technische Bundesanstalt, Germany,
S. L. Yaniv, A. Sawla, and M. Peters. 1991, 12p

Prepared in cooperation with Physikalisch-Technische Bundesanstalt, Brunswick (Germany, F.R.). Included in Jnl. of Research of the National Institute of Standards and Technology, v96 n5 p529-540 Sep/Oct

Keywords: \*Standards, Force(Mechanics), Interlaboratory comparisons, Static loads, Transducers, \*Force measurement, \*Force standards, Deadweight machines, US NIST.

A comparison of force measurements performed at the National Institute of Standards and Technology, USA, and at the Physikalisch-Technische Bundesanstalt, Germany is reported. The focus of the study was the intercomparison of the forces realized by the two Institutes rather than the measurement process. The transfer standards used in the comparison consisted of force transducers and associated readout instru-mentation. The results of the intercomparison reveal that over a range of 50 kN to 4.5 MN, the forces realized at NIST and at PTB compare favorably. For forces up to 900 kN the agreement is within + or - 40 ppm; above 900 kN the agreement is within + or - 100 ppm.

### General

PC A03/MF A01 AD-A227 806/7 AD-A227 806/7
National Inst. of Standards and Technology (NML),
Boulder, CO. Time and Frequency Div.
Cooled Ion Frequency Standard.
Annual rept. 1 Oct 89-31 Sep 90.
D. J. Wineland. 15 Sep 90, 17p
Contract N00014-90-F-0004

Keywords: Atomic spectroscopy, Cooling, Doppler effect, Electromagnetism, \*Frequency standards, High resolution, Ions, Laser applications, Radiation pressure, Residuals, Radiative transfer, Storage, Transitions, Traps, Penning Traps, Laser Cooling, Ion traps, Penning traps.

The purpose of this work is to develop techniques to overcome the fundamental limits of present frequency standards--the second order and residual first-order Doppler shifts. To this end suitable frequency refer-ence transitions are studied for ions which are stored on electromagnetic traps and cooled by radiation pressure to less than 1K. Keywords: Atomic spectroscopy; Doppler narrowing; Doppler shifts; Frequency stand-ards; High resolution spectroscopy; Ion storage; Laser spectroscopy; Penning trap; Laser cooling. (jhd)

AD-A242 029/7 PC A02/MF A01 National Inst. of Standards and Technology, Boulder,

Liquid and Solid Ion Plasmas. Annual rept. 1 Oct 90-31 Sep 91.
D. J. Wineland, and J. J. Bollinger. 15 Sep 91, 8p
Contract N00014-89-F-0020

Keywords: Angular momentum, Cooling, Distribution functions, Electromagnetic fields, Images, lons, Lasers, Plasmas(Physics), Solids, Spatial distribution, Spectroscopy, Temperature, Velocity, Laser cooling, Penning traps, \*lon plasmas.

Atomic ions which are stored in electromagnetic fields are an example of nonneutral plasmas. Laser techniques allow control of plasma angular momentum and provide plasma cooling to temperatures much less than 1K. Using imaging techniques, plasma spatial in-formation is achieved. Laser spectroscopic techniques

General

allow measurement of plasma velocity distribution functions. Liquid and solid behavior of ion plasmas is studied.

101,593

AD-A242 030/5 PC A02/MF A01 National Inst. of Standards and Technology, Boulder,

Cooled Ion Frequency Standard. Annual rept. 1 Oct 90-31 Sep 91. D. J. Wineland. 15 Sep 91, 8p Contract N00014-90-F-0004

Keywords: Doppler effect, \*Frequency standards, lons, Radiation pressure, Residuals, Transitions, \*Laser cooling, Penning traps, \*Atomic spectroscopy.

The purpose of this work is to develop techniques to overcome the fundamental limits of present frequency standards—the second order and residual first-order Doppler shifts. To this end we study suitable frequency reference transitions in ions which are stored on electromagnetic traps and cooled by radiation pressure to less than 1K.

101.594

#### PB90-244575

(Order as PB90-244526) Massachusetts Univ., Amherst. Dept. of Physics and

Astronomy.

Energy Levels of Atomic Aluminum with Hyperfine

Structure.

Quarterly rept. E. S. Chang. c1990, 7p Contract DNA-001-85-C-0022

Sponsored by Defense Nuclear Agency, Washington,

Included in Jnl. of Physical and Chemical Reference Data, v19 n1 p119-126 1990. Available from American Chemical Society, 1155 16th St., NW, Washington, DC 20036

Keywords: \*Atomic energy levels, Hyperfine structure, Electron transition, Ionization potentials, Spectra, \*Aluminum ions.

A new energy level table for AII has been constructed to include hyperfine structure from observations within the last decade. Improvement in accuracy over older tables is about an order of magnitude. The analysis of high-I Rydberg levels using the polarization formula results in a new value for the ionization potential which is 0.110/cm or five standard deviations above the old value. (Copyright (c) 1990 by the U.S. Secretary of Commerce.)

101 595

#### PB90-244583

(Order as PB90-244526)

Japan Atomic Energy Research Inst., Tokai.
Spectral Data and Grotrian Diagrams for Highly Ionized Iron, Fe VIII-XXVI.

Quarterly rept. T. Shirai, Y. Funatake, K. Mori, J. Sugar, W. L. Wiese, and Y. Nakai. c1990, 149p Sponsored by Department of Energy, Washington, DC.

Prepared in cooperation with Hiroshima-Denki Inst. of

Tech. (Japan), and National Inst. of Standards and Technology, Gaithersburg, MD. Included in Jnl. of Physical and Chemical Reference Data, v19 n1 p127-276 1990. Available from American Chemical Society, 115 16th St., NW, Washington, DC

Keywords: Transition probabilities, Atomic energy levels, Spectra, Tables(Data), Graphs(Charts), \*Iron ions, Multicharged ions, Grotrian diagrams, Oscillator strenaths.

Wavelengths, energy levels, level classifications, oscillator strengths, and atomic transition probabilities for the iron ions Fe VIII to Fe XXVI are critically reviewed and tabulated. Grotrian diagrams are also presented to provide graphical overviews. The literature has been surveyed to March 1988. (Copyright (c) 1990 by the U.S. Secretary of Commerce.)

#### 101.596 PB90-244666

(Order as PB90-244658) National Inst. of Standards and Technology (NML) Gaithersburg, MD. Center for Atomic, Molecular and Optical Physics. Energy Levels of Copper, Cu I through Cu XXIX. Quarterly rept.

J. Sugar, and A. Musgrove. c1990, 90p Included in Jnl of Physical and Chemical Reference Data, v19 n3 p527-616 1990. Available from American Chemical Society, 1155 16th St., NW, Washington, DC 20036.

\*Atomic energy levels. Spectra, Keywords: Tables(Data), \*Copper ions, Multicharged ions

The energy levels of the copper atom, in all stages of ionization for which experimental data are available, have been compiled. Ionization energies, either experimental or theoretical, and experimental g-factors are given. Leading components of calculated eigenvectors are listed. (Copyright (c) 1990 by the U.S. Secretary of Commerce.)

101.597 PB90-244690

(Order as PB90-244658)

Joint Inst. for Lab. Astrophysics, Boulder, CO.
Cross Sections and Swarm Coefficients for H+, H2+, H3+, H, H2, and H-in H2 for Energies from 0.1 eV to 10 keV.

Quarterly rept.

A. V. Phelps. c1990, 23p Included in Jnl. of Physical and Chemical Reference Data, v19 n3 p653-673 1990. Available from American Chemical Society, 1155 16th St., NW, Washington, DC 20036

Keywords: \*Collision cross sections, Momentum transfer, Excitation, Dissociation, \*Atom-molecule collisions, \*Molecule-molecule collisions, \*Ion-molecule \*Ion-molecule collisions, "Hydrogen ions 1 minus, "Hydrogen ions 1 plus, "Hydrogen ions 2 plus, "Hydrogen ions 3 plus, Charge exchange, Rotational states, Vibrational states, Swarm coefficients.

Graphical and tabulated data and the associated bibliography are presented for cross sections for elastic, excitation and ionization collisions of H(1+), H2(1+), H3(1+), H, H2, and H(1-) with H2 at laboratory energies from 0.1 to 10 keV. Where appropriate, drift velocities and reaction or excitation coefficients are calculated from the cross sections and recommended for use in analyses of swarm experiments and electrical discharges. Collisions of electronically excited states with H2 are not included. (Copyright (c) 1990 by the U.S. Secretary of Commerce.)

101,598

PB91-132290 PC A04/MF A01 National Inst. of Standards and Technology (NML), Gaithersburg, MD. Center for Radiation Research. Absorbed Dose Calibration of Ionization Chambers in a(60)Co Gamma-Ray Beam. Special pub. (Final). J. S. Pruitt. Oct 90, 56p NIST/SP-250/40

Also available from Supt. of Docs. as SN003-003-03034-1

Keywords: \*Ionization chambers, Radiation dosage, Cobalt 60, Calorimeters, Gamma rays, Water, \*Radiation doses, \*Calibration, Interlaboratory comparisons, Gamma dosimetry.

Measurement Service C.1 from the National Institute of Standards and Technology (NIST) publication SP 250 provides calibrations for customer-owned ionization chambers so that they may be used to determine absorbed dose to water in (60)Co gamma-ray beams. The calibrations are based on calorimetric measurement of absorbed dose to graphite in a graphite phantom. Transformation of the calibrations to a water phantom is made with a specially-designed graphite ionization chamber, and requires knowledge of photon mass attenuation coefficients and the perturbation of the graphite chamber in the water medium. The determination of these quantities is described in detail, along with the operational techniques normally used to transfer the calibration to customer-owned chambers. Appendix A lists experimental data used to test the photon-fluence scaling theorem. Appendices B, C, and D describe international comparisons of the chamber calibrations, and Appendix E shows a sample calibration report.

101.599

PB91-133900 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Quantum Metrology Div. Parity-Unfavored Transitions in Resonant Photoemission from Ar, Kr, and Xe: Experimental and Theoretical Results.

J. W. Cooper, D. W. Lindle, T. A. Carlson, D. R. Mullins, C. E. Beall, B. W. Yates, J. W. Taylor, and F. A. Grimm. 1990, 10p

Pub. in Jnl. of Electron Spectroscopy and Related Phenomena 51, p397-406 1990.

Keywords: \*Argon, \*Krypton, \*Xenon, Synchrotron radiation, Electron transitions, Auger electrons, Angular distribution, Reprints, \*Photoemission, Electron spectroscopy, High resolution.

High-resolution angle-resolved electron spectroscopy with synchrotron radiation has been used to study the angular distributions of resonant-Auger processes near the core-level thresholds Ar 2p, Kr 3d and Xe 4d. Angular-distribution parameters (beta) were measured for all resolved peaks in the electron spectra, and large negative values of beta were found for some peaks. A quantitative method for calculating the angular-distribution parameters is described and results of calculations for the Ar 2p(3/2) -> 4s resonant-Auger spectrum are compared with the experimental results.

101.600

PB91-134486 Not available NTIS National Inst. of Standards and Technology (NEL), Boulder, CO. Electromagnetic Technology Div High-Resolution, Tunneling-Stabilized Magnetic Imaging and Recording. Final rept.

J. Moreland, and P. Rice. 1990, 3p Pub. in Applied Physics Letters 57, n3 p310-312, 16 Jul

Keywords: \*Magnetic recording, Metal films, Iron, Reprints, Surface magnetism, Imaging techniques, High resolution, Scanning tunneling microscopy, Magnetic

The authors have used a scanning tunneling microscope (STM) to record and image magnetic regions on the surface of a hard disk. The usual rigid STM tip was replaced by a compliant magnetized Fe film tip. As a result, tunneling images were combinations of the surface topography and variations in the magnetic force between the Fe film tip and the disk surface. The authors believe that the recording process relied on maintaining the proximity of the magnetized Fe film tip near the disk surface. Apparently, the magnetic field was focused near the Fe film tip with sufficient intensity to change the surface magnetization of the disk. The authors have recorded spots on the disk within a 500 nm X 500 nm area. These spots were subsequently imaged with the same STM tip. Their best magnetic image resolution was 20 nm. The compliance of the Fe film tips was such that image contrast due to variation of the magnetic force on the tip corresponded to z motions of the piezoelectric translator as large as 50 nm.

101,601

PB91-134502 Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Thermophysics Div.
Thermal Conductivity of a Moderately Dense Gas.

C. A. Nieto de Castro, D. G. Friend, R. A. Perkins, and J. C. Rainwater, 1990, 8p

Pub. in Chemical Physics 145, p19-26 1990.

Keywords: \*Thermal conductivity, \*Gases, Nitrogen, Argon, Reprints, Lennard-Jones potential, Virial coefficients, Density dependence.

Recent extensive measurements of the thermal conductivity of argon and nitrogen have enabled us to evaluate the first density correction as a function of temperature and to compare it with a theoretical pre-diction. The prediction follows from a previously pub-lished microscopically based theory, which includes effects due to collisional transfer, collisions among three molecules, and monomer-dimer collisions. The first density correction was evaluated for a Lennard-Jones interaction potential. An ad hoc modification of the theory accounts for contributions to the thermal conductivity from internal degrees of freedom. The comparison shows good agreement over a wide range of temperatures.

101,602

PB91-134577

Not available NTIS

### General

National Inst. of Standards and Technology (NML), Boulder, CO. Thermophysics Div.

Thermal Conductivity and Heat Capacity of Gaseous Argon. Final rept.

H. M. Roder, R. A. Perkins, and C. A. Nieto de

Castro. 1989, 24p Pub. in International Jnl. of Thermophysics 10, n6 p1141-1164 Nov 89.

Keywords: \*Argon, \*Thermal conductivity, \*Thermal diffusivity, \*Specific heat, Gases, Reprints, Transient hot wire technique.

The paper presents new absolute measurements of the thermal conductivity and of the thermal diffusivity of gaseous argon obtained with a transient hot-wire instrument. The authors measured seven isotherms in the supercritical dense gas at temperatures between 157 and 324 K with pressures up to 70 MPa and densities up to 32 mol/L and five isotherms in the vapor at temperatures between 103 and 142 K with pressures up to the saturation vapor pressure. The instrument is capable of measuring the thermal conductivity with an accuracy better than 1% and thermal diffusivity with an accuracy better than 5%. Heat capacity results were determined from the simultaneously measured values of thermal conductivity and thermal diffusivity and from the density calculated from measured values of pres-sure and temperature from an equation of state. The heat capacities presented in the paper, with a nominal accuracy of 5%, prove that heat capacity data can be obtained successfully with the transient hot wire technique over a wide range of fluid states. The technique will be invaluable when applied to fluids which lack specific heat data or an adequate equation of state.

101.603 PB91-134643 Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Quantum Physics Div. Lunar Gravitational Wave Antenna Using a Laser

Interferometer.

Final rept. R. T. Stebbins, and P. L. Bender. 1990, 14p

Pub. in AIP Conference Proceedings 202, Physics and Astrophysics from a Lunar Base, NASA Workshop (1st), Stanford, CA., May 19-20, 1989, p188-201 1990.

Keywords: Angular resolution, Sensitivity, Reprints, \*Gravitational wave antennas, Laser interferometers, Lunar bases, Lunar surface.

A moon-based laser interferometer for detecting gravitational radiation could detect signals in the band 0.1 to 10,000 Hz. A preliminary evaluation of the noise budget for an optimistic antenna design is reported here and compared to that for other planned gravita-tional wave interferometers. Over most of the frequency range, the sensitivity is controlled by the thermal noise in the test mass suspensions. As pointed out by others, the most important role of a lunar antenna would be the improved angular resolution made possible by the long baseline to terrestrial antennas.

101.604 PB91-144360 PC A03/MF A01 National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Center for Computing and Applied Mathematics

Space Marching Difference Schemes in the Nonlinear Inverse Heat Conduction Problem.

A. S. Carasso. 21 Nov 90, 41p NISTIR-4482

Keywords: \*Conduction, \*Gun barrels, Nonlinear differential equations, Finite difference theory, One-dimensional calculations, Mathematical models, Heat transfer, Fourier analysis, Error analysis, III posed problems, Inverse problems.

The Lax-Richtmyer theory is used to study the error amplification properties of 18 space marching finite difference schemes, for the 1-D nonlinear inverse heat conduction problem. A non-dimensional parameter Omega, involving the time step Delta t, the effective thermal diffusivity alpha, and the distance I from the sensor to the active surface, provides a measure of the numerical difficulty of the inverse calculation. All 18 schemes are unstable and blow-up like 10(sup lambda Omega), where the constant lambda depends on the particular numerical method. However, there are substantial differences in the lambda's, and some newly constructed algorithms, employing forward time differences at nonadjacent mesh points, are shown to produce relatively low values of lambda. Using synthetic noisy data, a nonlinear reconstruction problem is considered for which Omega = 25. This problem simulates heat transfer in gun barrels when a shell is fired. It is shown that while most of the 18 schemes cannot recover the thermal pulses at the gun tube wall, two of the new methods provide reasonably accurate results. A tendency to underestimate peak values in fast, narrow thermal pulses, is also noted.

101,605 PB91-147116 PB91-147116 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div. Giant Resonances in the Transition Regions of the Periodic Table.

Final rept C. W. Clark, and T. B. Lucatorto. 1986, 15p Sponsored by Air Force Office of Scientific Research, Bolling AFB, DC.

Pub. in Giant Resonances in Atoms, Molecules, and Solids, p137-151 1986.

Keywords: \*Transition metals, \*Rare earth elements, \*Atomic orbitals, Giant resonance, Atomic structure, Reprints, Orbital collapse.

The behavior of the transition elements and the lanthanides is described in terms of an independent electron model. The properties of the transition elements and the lanthanides which are associated with orbital collapse are described in terms of an independent electron model. Special attention is focused on ele-ments at the beginning of the transition period, such as Cs, Ba, and La, to show that the dramatic changes in such properties as the photoabsorbtion can be ex-plained in terms of orbital collapse, provided one care-fully treats exchange and correlation effects. Theoretical models are compared with experimental results in isoelectronic and isonuclear systems.

101,606 PB91-147124 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Electricity Div.

Adjustment of the Fundamental Physical Constants: A Report of the CODATA Task Group on Fundamental Constants, 1986.

E. R. Cohen, and B. N. Taylor. 1986, 39p Sponsored by Rockwell International, Thousand Oaks, CA. Science Center Pub. in CODATA Bulletin, n63 39p 1986.

Keywords: \*Fundamental constants, Least squares method, Adjusting, Correction, Reprints.

The paper summarizes in some detail the 1986 leastsquares adjustment of the fundamental physical constants carried out by the authors under the auspices and guidance of the CODATA Task Group on Fundamental constants, and gives tables of recommended values of the constants for international use resulting from the 1986 adjustment. The 1986 CODATA set of values entirely replaces its immediate predecessor, that recommended for international use by CODATA in 1973. The latter was based on the 1973 least-squares adjustment of the fundamental constants which was also carried out by the authors under the auspices and guidance of the Task Group.

101,607 PB91-147173 PB91-147173 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Quantum Metrology Discovering to the Selective Excitation of Year Emission Control of Year Emission Control of Year Emission Selective Excitation of X-ray Emission Spectra.

Final rept.
P. L. Cowan. 1990, 7p
Pub. in Physica Scripta T31, p112-118 1990.

Keywords: \*X ray spectra, Synchrotron radiation, X ray absorption, X ray fluorescence, Emission spectra, Excitation, Reprints.

While X-ray emission spectroscopy is a relatively old technique, it takes on important new characteristics when samples are selectively excited by a carefully prepared beam of X-rays. The method is made practical by the availability of synchrotron radiation sources and it extends the capabilities of the traditional technique. Both the energy and the polarization of the excitation X-rays can have significant effects on the emission X-rays can have significant effects on the emission of the excitation X-rays can have significant effects on the emission of the excitation X-rays can have significant effects on the emission of the excitation of the excitat sion spectra. Selective control of these parameters can provide specific information on both the electronic structure and the atomic structure of molecules or solids. Examples of the new types of studies include: satellite free X-ray emission, multi-vacancy excitation, polarized X-ray excitation and emission, and state selective excitation of neutral atoms and molecules.

101.608

PB91-147249 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Ionizing Radiation Div.

Preparation and Properties of Monomolecular

Films for Use as Radioactive Source Mounts. Final rept.

L. J. Dobrilovic, M. Simovic, D. J. Bek-Uzarov, J. M. R. Hutchinson, and W. B. Mann. 1988, 7p Pub. in Applied Radiation and Isotopes 39, n9 p999-1005 1988.

Keywords: \*Monomolecular films, \*Radioactivity, \*Mountings, Chemisorption, Adsorption, Reprints, Calcium stearate, Multilayers.

The physical properties of the calcium-stearate monomolecular layer have been examined using an automatic torsion balance. These layers were obtained by adsorption of Ca(2+) ions from 0.0001 M CaCl2 onto the stearic-acid monomolecular layer. The introduction also briefly reviews previous work on the preparation of monomolecular layers and their use, for some 50 years, for radioactivity measurements.

101.609

PB91-147355 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Center for Radiation Research. Electrofission in the Quasifree and Delta Regions. Final rept.

K. Hansen, J. O. Adler, K. I. Blomqvist, D. Nilsson, A. Sandell, B. Schroder, W. R. Dodge, J. W. Lightbody, J. S. Connelly, F. W. Hersman, W. Kim, and M. Leuschner. 1990, 6p Pub. in Physical Review C 41, n4 p1619-1624 Apr 90.

Keywords: \*Uranium 238, \*Uranium 233, \*Fission cross sections, \*Electrofission, MeV range 100-1000,

The coincident electrofission (e,e'f) cross sections of (233,238)U were measured in the excitation range 150-550 MeV. The probability of fission was found to be near unity in the delta resonance region (250-550 MeV), but less than unity in the quasifree scattering region (150-250 MeV). The data are analyzed with a model based on the quasifree and delta reaction mechanisms. An excitation energy of 25 MeV is found for the residual nucleus in the quasifree region and over 40 MeV in the delta region.

101.610

PB91-147462 PB91-147462 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Atomic and Plasma Radiation Div. Transitions and Energy Levels for Cu-Like Yb(41+), Ta(44+), and U(63+).

D. R. Kania, B. J. MacGowan, C. J. Keane, C. M. Brown, and J. O. Ekberg. 1990, 4p Sponsored by Department of Energy, Washington, DC. Pub. in Jnl. of the Optical Society of America B 7, n10 p1993-1996 Oct 90.

Keywords: \*Ytterbium ions, \*Tantalum ions, \*Uranium ions, \*Atomic energy levels, \*Electron transitions, Plasma spectra, Multicharged ions, Soft x rays, Laserproduced plasma, Reprints.

Transitions from the n = 4.5, and 6 excited levels of the Cu-like ions Yb(41+), Ta(44+), and U(63+) were observed in the spectra from plasmas that were produced by one or two beams of the Nova laser. Wavelengths in the range 9-140 A were measured with an uncertainty of + or -0.015 A and were compared with previously measured and predicted wavelengths. The energy levels were derived from the observed wavelengths.

101.611

Not available NTIS PB91-147496 National Inst. of Standards and Technology (NEL), Boulder, CO. Electromagnetic Technology Div. Global Stability of the Chaotic State Near an Interior Crisis. Final rept.

R. L. Kautz. 1989, 20p Contract N00014-85-F-0085 Sponsored by Office of Naval Research, Arlington, VA. Pub. in Structure, Coherence and Chaos in Dynamical Systems, p207-226 1989.

Keywords: \*Chaos, Josephson junctions, Thermal noise, Attractors, Stability, Reprints.

In dissipative systems, chaotic trajectories are locally unstable in that they show a sensitive dependence on initial conditions but globally stable in that they are represented by attractors. The global stability of the chaotic state is examined in the neighborhood of an interior crisis using the rf-biased Josephson junction as an example. A measure of global stability is developed by considering the response of the system to thermal noise. In the presence of noise, the system occasionally escapes from the region of state space containing the attractor and the temperature dependence of the average escape time is characterized by an activation energy. The activation energy is a useful measure of the global stability of the chaotic state, being analogous to the barrier height for a particle in a potential

101.612 PB91-147587 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Center for Radiation Research. Possible (e,e'2N) Studies at CEBAF.

Final rept.

J. W. Lightbody. 1988, 9p Pub. in Proceedings of Workshop on Perspectives in Nuclear Physics at Intermediate Energies (3rd), Trieste, Italy, May 18-22, 1987, p455-473 1988.

Keywords: \*Knock-out reactions, \*Electron scattering, CEBAF accelerator, High energy particles, Spectrometers, Hadrons, Reprints.

Multi-hadron knockout by high energy electron scattering will be one of the high priority experimental programs at CEBAF. The motivation for such reaction studies has both an experimental and theoretical side and is discussed herein. The equipment required for such studies, the kinematics employed, estimates of counting rates, and related issues are also discussed.

101,613 PB91-147959 PB91-147959 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Center for Radiation Research. Muon Sticking in Catalysed d-t Fusion: Nuclear Resonance Effect.

Final rept. J. Rafelski, B. Muller, M. Danos, G. Velarde, and E.

Minguez. 1987, 6p
Pub. in Proceedings of International Conference on

Emerging Nuclear Energy Systems (4th), Madrid, Spain, June 30-July 4, 1986, p383-388 1987.

Keywords: \*Muon-catalyzed fusion, Deuteron reactions, Triton reactions, Reprints, Nuclear resonance.

The kinetic energy of a muon attached to the recoiling particle in d-t fusion reduces the energy available in the nuclear fusion channel by about (90 + or - 50)deV.) The highly resonant d-t reaction amplitude is detuned and therefore the reaction channel is further suppressed in comparision to the nonsticking reaction.

PB91-148684 Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Quantum Physics Div.

Close-Coupling Calculation for the (2)(Sigma sub u)(+) State of (H sub 2)(-). Final rept.

T. Gorczyca, and D. W. Norcross. 1990, 7p Grant NSF-PHY86-04504

Sponsored by National Science Foundation, Washington, DC

Pub. in Physical Review A 42, n9 p5132-5138, 1 Nov

Keywords: \*Hydrogen, Molecular structure, Negative ions, Bound state, Reprints.

The authors demonstrate the utility of the close-coupling approximation, usually applied to scattering problems, for calculations of molecular bound states. Their primary test case is the doublet Sigma (sub u)(sup +) state of H2(1-). While limited to Hartree-Fock accuracy, their analysis of this resonant state within the bound region parallels closely the results from more precise quantum-chemical calculations. Specifically, the crossing between the neutral and negative-ion curves occurs at an internuclear separation of 3.025 a.u. in their calculation, in good agreement with a multireference configuration-interaction approach of previous authors. The shape and total energy of the anion

curve, when corrected for by the correlation energy of the target at the crossing, is also in good agreement with earlier results. The method is then extended into the unbound or resonant-state region by studying the shape-resonance behavior of scattering eigenphase

PB91-148692 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Quantum Metrology Group.

Determination of the Neutron Mass and Implica-

tions for Fundamental Constants. G. L. Greene, E. G. Kessler, M. S. Dewey, and R. D.

Deslattes. 1987, 5p
Pub. in Proceedings of International Conference on
Neutron Physics, Kiev, Ukraine, USSR, September 21-25, 1987, p76-80

Keywords: Quantum electrodynamics, Fundamental constants, Rest mass, Reviews, Tests, Reprints,

The neutron mass, while not well understood theoretically, is known to quite high accuracy by a combination of absolute gamma ray spectroscopy and high accura-cy mass spectroscopy. A review of the current experi-mental status of the neutron mass is given, along with a discussion of the prospects for improvement in the near future. The implication of these results for the fundamental constants as well as for tests of QED is briefly reviewed.

101,616 PB91-148718 Not available NTIS National Inst. of Standards and Technology (NEL), Boulder, CO. Thermophysics Div. Anisotropic Structure of a Simple Liquid.

Final rept.

H. J. M. Hanley. 1988, 16p Sponsored by Department of Energy, Washington, DC.

Office of Basic Energy Sciences.
Pub. in Proceedings of the Winter Meeting on Statistical Physics Lectures on Thermodynamics and Statistical Mechanics (17th), Oaxtepec, Mexico, January 5-8, 1988, p109-124.

Keywords: \*Non-Newtonian fluids, Couette flow, Structure factors, Reprints, Molecular dynamics.

Non-Newtonian behavior in a sheared simple fluid is reviewed briefly. The author points out that such behavior is more often associated with fluids of very complex structure, such as polymers. The concept of the Maxwell relaxation time is introduced and it is shown that the product of the time and a shear rate is a key parameter that indicates if a fluid will display non-New-tonian characteristics, regardless of molecular structure. The author discusses the distorted structure factor of a dense two-dimensional soft disk liquid undergoing Couette flow. The structure factor is determined experimentally by light scattering from the output of a nonequilibrium molecular dynamic simulation. The distorted pair correlation function is also discussed.

101,617 PB91-149203 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Atomic and Plasma Radiation Div. Precise Experimental Test of Calculated Two-Electron Lamb Shifts in Helium.

Final rept. C. J. Sansonetti, J. D. Gillaspy, and C. L. Cromer.

1990, 4p Pub. in Physical Review Letters 65, n20 p2539-2542, 12 Nov 90.

Keywords: \*Helium, \*Lamb shift, Quantum electrodynamics, Electron transitions, Metastable state, Laser spectroscopy, Atomic energy levels, Tests, Reprints.

The authors have measured the wave number of the (4)He 2 singlet S -> 3 singlet P transition by Doppler-free spectroscopy in a metastable helium beam. The result, 19931.924794(45)/cm, represents an order of magnitude improvement over previous measurements and provides a sensitive test of two-electron QED effects. The result shows an unexpectedly large deviation from theoretical prediction. The authors derive improved term values for a number of low-lying helium levels. All levels with n=2 show significant deviations from theory that are correlated with the size of calculated two-electron contributions to the Lamb shifts.

101,618 PB91-149245

Not available NTIS

National Inst. of Standards and Technology (NML), Boulder, CO. Quantum Physics Div.

Nonresonant Charge Transfer in the Threshold Region for (3)He(+) + (4)He(sub <-sup->) (3)He + (4)He(+). Final rept.

M. M. Schauer, S. R. Jefferts, and G. H. Dunn. 1990,

Grant NSF-PHY86-04504 Sponsored by National Science Foundation, Washing-

ton, DC Pub. in Physical Review A 42, n9 p5332-5337, 1 Nov

Keywords: \*Helium, \*Charge transfer, Isotope effects, Helium 3, Helium 4, Cryogenics, Reprints.

Measurements of the ratio of the rate coefficient for charge transfer between (3)He(1+) and (4)He to that for the reverse process have been made in the temperature range 8 K approx = or < T approx = or < 80 K. A 1.1-meV difference in the ionization potential of these species leads to an endothermicity in the forward direction of the reaction, and these experiments constitute the only measurements of a threshold resulting from such á small endothermicity. In addition, a limited number of direct measurements of the rate coefficients for these processes have been made and are included here. The measurements were done in a cooled Penning trap using Fourier transform spectroscopy of the axial trapping frequency. The measurements are compared to theoretical estimates.

101,619 PB91-149971 Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Quantum Physics Div.

Optical Potential Approach to Electron and Positron Scattering from Noble Gases. 2. Neon. Final rept.

K. Bartschat, R. P. McEachran, and A. D. Stauffer. 1990, 7p Pub. in Jnl. of Physics B: Atomic and Molecular Phys-

ics 23, p2349-2355 1990.

Keywords: \*Electron-atom collisions, \*Positron-atom collisions, \*Neon, Electron scattering, Differential cross sections, Total cross sections, Optical models,

The authors have extended their previous work on an optical potential method to electron and positron scattering from neon. In addition, they have modified the approach to include the diagonal potentials previously neglected. This required the use of a numerical form of the Green function. Comparison with recent experimental measurements with positrons indicates the ne-cessity of including absorption effects at higher energies, although these effects appear to be smaller for neon than they were for argon. At energies just above the inelastic excitation thresholds, however, the picture is not so clear at the moment.

101.620

PB91-150011 Not available NTIS National Inst. of Standards and Technology (MSEL),

Gaithersburg, MD. Reactor Radiation Div.
Nonlocal Phase Shifts Induced by Static Electric
Fields in Neutron Interferometers When the Path-**Enclosed Charge Vanishes.** 

Final rept.

R. C. Casella. 1990, 4p Pub. in Physical Review Letters 65, n18 p2217-2220, 29 Oct 90.

Keywords: Electric fields, Phase shift, Reprints, \*Neutron interferometry.

An experiment, analogous to that of Cimmino et al., is proposed to measure the phase shift induced by static electric fields on the passage of neutrons through an interferometer when the path-enclosed linear charge density is zero. A finite shift is predicted and discussed in light of the Aharonov-Casher result.

101.621

PB91-158634 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Center for Basic Standards.

Accurate Spectroscopy In the X-ray Region.

Final rept.

R. D. Deslattes. 1988, 8p

Pub. in Nuclear Instruments and Methods in Physics Research B31, n1-2 p51-58 Apr 88.

#### General

Keywords: \*X ray spectroscopy, Multicharged ions, Heavy ions, Precision, Accuracy, Reprints.

There is currently not only keen interest in accurate spectroscopy of one- and two-electron ions but also the by now well-founded hope that these spectra can be produced under conditions where Doppler and spectator electron problems are under adequate control. These developments will require that one confront problems of wavelength normalization at a more refined level than has been necessary in the past. The report briefly outlines the present-day situation in the case of using normal x-ray lines as references, and the steps which might be taken to transcend limitations inherent in the approach.

101,622

PB91-158881 Not available NTIS National Bureau of Standards (NML), Gaithersburg,

National Bureau of Standards (INVIL), Galdielsburg, MD. Molecular Spectroscopy Div. Explicit Mapping of the Set of Dynamical Symmetries onto the Set of Equivalent Lagrangians for Systems with One Degree of Freedom. Final rept.

C. Leubner, and M. A. M. Marte. 1986, 6p Pub. in Physics Letters A 117, n2 p67-72, 28 Jul 86.

Keywords: \*Mechanics, Lagrangian functions, Dynamics, Reprints, One degree of freedom.

For newtonian systems with one degree of freedom, for which the existence of a relationship between the dynamical symmetries of the equation of motion and its equivalent lagrangian descriptions is well known, an explicit method is given for establishing the lagrangian associated with any particular dynamical symmetry.

101,623

PB91-159236 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Electricity Div. Preface to Book Entitled Nonequilibrium Effects

in Ion and Electron Transport'.

Final rept.

R. J. Van Brunt. 1990, 2p Pub. in Nonequilibrium Effects in Ion and Electron Transport, pv-vi 1990.

Keywords: \*Gas discharges, \*Electron transport, Breakdown(Electronic threshold), Electric discharges, \*Electron\_transport Collision cross sections, Electron collisions, Atomic collisions, Reprints, \*lon transport, Swarm seminar.

The volume presents the contributions of the participants in the Sixth International Swarm Seminar, held August 2-5, 1989, at the Webb Institute in Glen Cove, New York. The Swarm Seminars are traditionally held New York. The Swarm Seminars are traditionally held as relatively small satellite conferences of the International Conference on the Physics of Electronic and Atomic Collisions (ICPEAC) which occurs every two years. The 1989 ICPEAC took place in New York City prior to the Swarm Seminar. The focus of the Swarm Seminars has been on basic research relevant to understanding the transport of charged particles, mainly electrons and ions, in weakly ionized gases. This is a field that tends to bridge the gap between studies of field that tends to bridge the gap between studies of fundamental binary atomic and molecular collision processes and studies of electrical breakdown or discharge phenomena in gases. Topics included in the 1989 seminar ranged the gamut from direct determinations of charged-particle collision cross sections to use of cross sections and swarm parameters to model the behavior of electrical gas discharges.

PB91-159251 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Office of Standard Reference Data.

Steam Tables. Final rept.

H. J. White. 1987, 10p

Pub. in Encyclopedia of Physical Science and Technology, v13 p328-337 1987.

Keywords: \*Steam tables(Thermodynamics), Physical properties, Encylopedias, Reprints.

Steam tables are defined and a brief history of the development is given. Emphasis is based on steam tables receiving international acceptance, i.e., those of the International Association for the Properties of Steam (IAPS) and its predecessors. A listing of current releases from IAPS, including automated versions and archival decuments, supporting those releases are archival documents supporting those releases, are available.

101.625

PB91-159285 Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Time and Frequency Div. Progress at NIST on Absolute Frequency Stand-

ards Using Stored Ions.

Final rept.

Final rept.

D. J. Wineland, J. C. Berquist, J. J. Bollinger, W. M. Itano, D. J. Heinzen, S. L. Gilbert, C. H. Manney, M. G Raizen, and C. S. Weimer. 1990, 6p See also PB90-188616. Sponsored by Office of Naval Research, Arlington, VA., and Air Force Office of Scientific Research, Bolling AFB, DC. Pub. in Proceedings of European Frequency and Time Forum (4th), Neuchatel, Switzerland, March 13-15, 1990, p267-272.

Keywords: \*Atomic clocks, \*Frequency standards, \*Standards, \*Ion storage, Atomic spectroscopy, High resolution, Laser spectroscopy, Beryllium 9, Mercury 199, Reprints, Ion storage, Penning traps, Paul traps, Laser cooling.

Experiments at NIST, whose goal is to realize frequency standards of high accuracy using stored ions, are briefly summarized. In one experiment, an rf oscillator is locked to a nuclear spin-flip hyperfine transition in (9)Be(1+) ions which are stored in a Penning trap and sympathetically laser-cooled. Uncertainty in Doppler shifts is estimated to be less than  $5 \times 10$ (sup -15). In a second experiment, a stable laser is used to probe an electric experiment, a stable laser's used to proble the electric quadrupole transition (frequency = 1.07 x 10(sup 15) Hz) in a single laser-cooled (199)Hg(1+) ion stored in a Paul trap. The measured Q value of the transition is approximately 10(sup 13).

101,626 PB91-159301 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.

Photoionization and Collisional Ionization of Excited Atoms Using Synchrotron and Laser Radiations.

Final rept. F. J. Wuilleumier, D. L. Ederer, and J. L. Picque.

1987, 90p Pub. in Advances in Atomic and Molecular Physics 23, p197-286 1987.

Keywords: \*Excited states, \*Photoionization, Laser radiation, Synchrotron radiation, Autoionization, Atoms, Reprints, Collisional ionization.

The article is devoted to a description of various ionization processes which may be studied in excited atoms. Some of these processes are: photoionization, autoionization, and collisional ionization. The development of the field has been accelerated by combining tunable lasers, which excite the atomic species, with synchrotron radiation, which probes the excited atoms. The authors concentrate on the two-step photoionization in free atoms where one electron is promoted to an outer orbital and another is promoted either to a highly excited state which subsequently autoionizes, or to a continum state.

101.627

Final rept.

PB91-161976 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Statistical Engineering Div. Cross-Validation Procedure for Stopping the EM

Algorithm and Deconvolution of Neutron Depth Profiling Spectra.

K. Coakley, 1991, 7p Pub. in IEEE (Institute of Electrical and Electronics Engineers) Transactions on Nuclear Science 38, n1 p9-15 Feb 91.

Keywords: \*Neutron spectra, \*Image reconstruction, Stopping rules(Mathematics), Iterations, Reprints, Emission tomography, EM algorithm, Deconvolution, Depth profiles.

The iterative EM algorithm is used to deconvolve neutron depth profiling spectra. Because of statistical noise in the data, artifacts in the estimated particle emission rate profile appear after too many iterations of the EM algorithm. To avoid artifacts, the EM algorithm. rithm is stopped using a cross-validation procedure. The data are split into two independent halves. The EM algorithm is applied to one half of the data to get an estimate of the emission rates. The algorithm is stopped when the conditional likelihood of the other half of the data passes through its maximum. The roles of the two halves of the data are then switched to get a second estimate of the emission rates. The two estimates are then averaged.

101,628

PB91-162123 Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Time and Frequency Div. Quantum Optics of Single, Trapped Ions.

W. M. Itano, J. C. Bergquist, F. Diedrich, and D. J. Wineland. 1990, 5p Sponsored by Air Force Office of Scientific Research, Bolling AFB, DC., and Office of Naval Research, Arlington, VA. Pub. in Coherence and Quantum Optics VI, p539-543

1990

Keywords: \*Mercury ions, \*Ion storage, \*Quantum optics, Trapping(Charged particles), Photons, Reprints, Laser cooling, Ion traps.

Quantum jumps in laser-cooled, trapped, mercury ions were observed. These quantum jumps were used to infer some quantum properties of the electromagnetic field, such as photon antibunching and sub-Poissonian photon statistics. A single mercury ion was cooled to the ground (zero-point) energy in the harmonic effective potential of the trap.

101.629

PB91-167205 PB91-167205 PC A03/MF A01 National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Center for Computing and Applied Mathematics.

Uncertainty and Accuracy in Physical Measure-

Richards Special pub. (Final). H. H. Ku. Dec 90, 14p NIST/SP-805 Also available from Supt. of Docs.

Keywords: \*Uncertainty, \*Accuracy, Measurement, Recommendations, Standards, Calibration.

The formulation of the 'uncertainty' of a reported value always involves a certain degree of arbitrariness, de-pending primarily on how the value is going to be used. Currently there are at least two schools of thought on the subject: physicists interested in detecting differences among result are in favor of the recommendations of the International Bureau of Weights and Measures (BIPM/CIPM 1981), whereas those involved in calibration work and routine measurements follow the orthodox method (see e.g., NBS Special Publication 644). In the note, the suggestion is made to use the word 'accuracy/inaccuracy' for standards that follow BIPM's recommendation, and the word 'uncertainty' for standards that follow the orthodox method. It is believed that the use of different terms for distinct pur-poses will resolve some of the basic difficulties facing international groups who are attempting to write their own standards

101,630

PB91-174722 Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Quantum Physics Div.

Gyroscope-Weighing Experiment Revisited -- with a Null Result.

Final rept. J. E. Faller, W. J. Hollander, P. G. Nelson, and M. P.

McHugh. 1990, 5p Pub. in Proceedings of Recontre de Moriond New and Exotic Phenomena (25th), Les Arcs, Savoie, France, January 20-27, 1990, p197-201.

Keywords: \*Weight reduction, \*Gyroscopes, Spinning(Motion), Experimentation, Gravity, Reprints.

A recent experiment that reported finding an anomalous weight reduction for a spinning gyroscope weighed on a pan balance has been repeated during six days in the laboratory. No anomalous weight changes of the magnitude reported, were found that depended on rotor speed and/or its direction of rotation about the vertical axis.

101,631

PB91-174748 Not available NTIS National Inst. of Standards and Technology (NEL), Boulder, CO. Electromagnetic Technology Div.

Anomalous Magnetoresistance in Al/Al-Alloy Composite Conductors.

Final rept. F. R. Fickett, and C. A. Thompson. 1990, 8p Sponsored by Wright Research and Development Center, Wright-Patterson AFB, OH.

Pub. in Advances in Cryogenic Engineering (Materials), v36 p671-678 1990.

Keywords: \*Magnetoresistance, Electric conductors, Composite materials, Aluminum, Cryogenics, Anomalies. Reprints.

The transverse magnetoresistance of several composite conductors containing a large single filament of pure aluminum in a matrix of Al-Fe-Ce has been measured at 4 K to fields of 10 T. The magnetoresistance (delta R/R) of the composite is very large, rising to 55 in the 'worst' case. Previous measurements on pure polycrystalline aluminum have always shown a rapidly saturating behavior with a very small linear component; delta R/R rarely exceeds a value of 5-6. In addition, the magnetoresistance of the composite samples shows a structure as the field is rotated around the current axis.

101,632 PB91-174755 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Ionizing Radiation Div. New Test of Quantum Mechanics: Is Planck's Con-

stant Unique.

E. Fischbach, G. L. Greene, and R. J. Hughes. 1991,

Sponsored by Department of Energy, Washington, DC. Pub. in Physical Review Letters 66, n3 p256-259, 21

Keywords: \*Quantum mechanics, \*Conservation laws, \*Plancks constant, Fundamental constants, Invariance, Tests, Reprints.

The possibility that different realms of physics are described by distinct quantization constants is considered. From the consistency of existing data, the authors infer limits on the differences between hypothetically distinct quantization constants for different elementary particles. Since the existence of multiple Planck constants implies violations of space-time symmetries, these limits may be viewed as precise tests of fundamental conservation laws, including the conservation of linear momentum and energy.

101,633 PB91-174888 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Surface Science Div. Instrumentation of X-ray Beam Lines with PIN

**Diode Detectors.** Final rept. T. J. Jach. 1990, 4p

Pub. in Nuclear Instruments and Methods in Physics Research A299, p76-79 1990.

Keywords: \*Synchrotron radiation sources, \*X-ray detection, \*PIN diodes, Silicon diodes, Photodiodes, Performance, Reprints, Beamlines.

Much of the X-ray work on synchrotron-radiation beam lines is still done using ion chambers as detectors. Silicon PIN photodiodes offer considerable advantages over ion chambers for many applications. In addition to greater efficiency over a wide energy range (1-20 keV), they possess a flat configuration, large areas, an absence of bias requirements, high dynamic range, and compatability with ultrahigh vacuum. The researchers have characterized the properties of several commercial PIN photodiodes at X-ray energies, have had diodes commercially produced which were specialized for use in synchrotron beam lines, and have produced new photodiode devices for synchrotron-radiation applications. The performance of these devices was reviewed over extended periods of time in beam-line control and as detectors in experiments.

Not available NTIS PB91-174987 National Bureau of Standards (NEL), Gaithersburg, MD. Precision Engineering Div. Optical Levitation of Single Particles.

T. R. Lettieri, 1988, 10p

Final rept

Pub. in Proceedings of Scientific Conference on Obscuration and Aerosol Research, Edgewood, MD., June 26-30, 1987, p305-314 1988.

Keywords: \*Radiation pressure, \*Levitation, Laser radiation, Drops(Liquids), Microspheres, Reprints, \*Optical levitation

Experimental techniques are presented for optically levitating single particles using laser radiation pres-

101,635 PB91-175083 Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Quantum Physics Div.

Gravitational Radiation Observations on the Moon. Final rept

R. T. Stebbins, J. W. Armstrong, P. L. Bender, R. W. P. Drever, R. W. Hellings, and P. R. Saulson. 1990,

Pub. in Proceedings of NASA Workshop on Astrophysics from the Moon, Annapolis, MD., February 5-7, 1990, p637-646.

Keywords: \*Gravitational wave antennas, \*Lunar observatories, Laser interferometry, Lunar bases, Reprints

A Laser-Interferometer Gravitational-Wave Observatory (LIGO) is planned for operation in the United States, with two antennas separated by several thousand kilometers. Each antenna would incorporate laser interferometers with 4 km arm lengths, operating in vacuum. The frequency range covered initially would be from a few tens of Hz to a few kHz, with possible extension to lower frequencies later. Similar systems are likely to be constructed in Europe, and there is a possibility of at least one system in Asia or Australia. It will be possible to determine the direction to a gravitational wave source by measuring the difference in the arrival times at the various antennas for burst signals or the phase difference for short duration nearly periodic signals. The addition of an antenna on the Moon, operating in support of the Earth-based antennas, would improve the angular resolution for burst signals by about a factor 50 in the plane containing the source, the Moon, and the Earth.

101.636 PB91-175265 Not available NTIS National Bureau of Standards (NML), Gaithersburg,

MD. Ionizing Radiation Div.
Status of Beta-Particle Calibration Studies at NBS. Final rept.

C. G. Soares, and J. S. Pruitt. 1987, 3p Pub. in Proceedings of Department of Energy Work-shop on Beta Measurements, Albuquerque, NM., January 23-24, 1986, p169-171 1987.

Keywords: \*Ionization chambers, \*Beta detection, \*Beta sources, \*Test facilities, \*Calibration, Radiation protection, Electron beams, US NBS, Reprints.

A calibration facility for beta-particle instruments and sources used in radiation protection has been established at the National Bureau of Standards (NBS). The facility consists of standardized beta-particle sources and extrapolation ionization chambers for the accurate measurement of beta-particle absorbed dose. The facility also includes a series of nearly monoenergetic electron beams for measurement of instrument re-sponse functions. A service which has been established for the calibration of beta-particle sources and transfer-quality ionization chambers is described. The latest improvements to the monoenergetic electron facility are also discussed.

101,637 PB91-175273 Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Quantum Physics Div.

Test of Newton's Inverse Square Law of Gravity Using the 300 m Tower at Erie, Colorado: Newton Vindicated on the Plains of Colorado.

Final rept. C. C. Speake, T. M. Niebauer, M. P. McHugh, P. T. Keyser, J. E. Faller, J. Y. Curz, J. C. Harrison, J. Makinen, and R. B. Beruff. 1990, 8p

Pub. in Proceedings of Rencontre de Moriond New and Exotic Phenomena (25th), Les Arcs, Savoie, France, January 20-27, 1990, p255-262.

Keywords: \*Gravitation, \*Gravity, Tests, Reprints, Meteorological towers, Inverse square laws, Newton laws.

A 300-m meteorological tower was used to measure gravity at eight different heights above the surface of the earth. The observed gravity values were corrected

for tides and gravimeter screw error. Also, tests were performed to look for systematic effects due to tower motion. The resulting values are compared to values predicted by Newton's inverse-square law from upward continuation of surface gravity. The result places new constraints on any non-Newtonian interac-

101,638 PB91-175364 Not available NTIS National Inst. of Standards and Technology (PL), Gaithersburg, MD. Atomic Physics Div. Spectrum and Energy Levels of the Xenonlike Ion

Ce V. Final rept.

A. Redfors, and J. Reader. 1991, 7p Sponsored by Department of Energy, Washington, DC. Pub. in Physical Review A 43, n5 p2367-2373, 1 Mar

Keywords: \*Cerium ions, \*Energy levels, \*Ultraviolet spectra, Vacuum ultraviolet radiation, Multicharged ions, Hartree-Fock approximation, Reprints.

The spectrum of four-times ionized cerium Ce v has been observed with a sliding-spark discharge and a 10.7-m normal-incidence vacuum spectrograph. A total of 107 lines have been classified as transitions between 51 energy levels. All levels of the 5p(6), 5p quintet 4f, 5p quintet 5d, 5p quintet 6s, 5p quintet 6p, and 5p quintet 6d configurations have been determined. Because of collapse of the 4f shell, the 5p guintet 4f configuration is situated well below 5p quintet 5d. Ab initio calculations and least-squares fits of the energy parameters to the experimental energy levels are reported. The ionization energy is revised to 527100 + or - 2000/cm (65.35 + or - 0.25 eV).

PB91-175380 Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Quantum Physics Div.

Search for a Composition Dependent Force Using a Liquid-Supported Torsion Balance. Final rept

M. P. McHugh, P. T. Keyser, and J. E. Faller. 1990, Pub. in Proceedings of the Recontre de Moriond New

and Exotic Phenomena (25th), Les Arcs, Savoie, France, January 20-27, 1990, p233-236.

Keywords: \*Basic interactions, Torsion balances, Lead(Metal), Copper, Reprints, \*Fifth force, Eotvos experiment.

Current efforts are discussed to search for an intermediate range composition dependent interaction, using a liquid-supported torsion balance containing a Pb-Cu composition dipole. The mass inhomogeneity of the basement laboratory serves as the source for the interaction. The expected sensitivity and preliminary results are presented.

101.640 PB91-175430 Not available NTIS National Bureau of Standards (NEL), Boulder, CO. Chemical Engineering Science Div.

Saran Carbon Cryogenic Regenerator for Liquid

Final rept. L. V. Munukutla, J. A. Jones, and R. Radebaugh, 1988, 10p

Pub. in Proceedings of Interagency Meeting on Cryocoolers, Monterey, CA., August 17, 1988, p109-118.

Keywords: \*Carbon, \*Regenerators, \*Liquid helium, Cryogenics, Adsorption, Heat exchangers, Thermal conductivity, Reprints.

A promising solution to the problems of regenerator ineffectiveness in the 4K to 15K region is the use of saran carbon with adsorbed helium as the regenerator material. Preliminary measurements indicate that this material has a higher volumetric specific heat than any other known material in the 4K to 15K temperature range. Furthermore, the estimated thermal conductivity of saran carbon is low enough to permit its use as a continuous matrix between the hot and cold ends of the regenerator, but it does not adversely affect the longitudinal conduction heat loss along the regenerator length. An NBS computer regenerator program has been used to show that a saran carbon/ adsorbed helium, parallel-plate geometry regenerator is likely to be superior to any other known regenerator for cooling in the 4K to 15K temperature region.

#### General

101,641 PB91-175497 Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Quantum Physics Div.

Spin-Dependent Electron-Impact Excitation of Sodium. Final rept.

Number 1990, H. L. Zhou, B. L. Whitten, G. Snitchler, D. W. Norcross, and J. Mitroy. 1990, 6p Contract DE-Al05-86ER53237

Sponsored by Department of Energy, Washington, DC. Office of Basic Energy Sciences.
Pub. in Physical Review A 42, n7 p3907-3912, 1 Oct

Keywords: \*Electron scattering, \*Sodium, Atomic energy levels, Electron spin, Excitation, EV range 01-R matrix, Reprints.

The spin-dependent cross sections for electron excitation of the 3p level of sodium at energies just above threshold are studied using the R-matrix approach. In addition to the total cross section for excitation, the authors present results for the excitation cross sections as a function of the change in the spin and orbital angular-momentum projection of the target. Calculations were made in the four-(3s,3p,4s,3d), five-(+4p,4d) approximations, for electron energies ranging from threshold to 4.0 eV. The results are compared with other calculations and with the recent experimental results of Han, Schinn, and Gallagher (Phys. Rev. A 38,535 (1988)).

101 642 PB91-175513 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.

Of What Use Is Basic Research.

Final rept.

. B. Lucatorto. 1987, 1p Pub. in Candela Wavelength, p5 1987.

Keywords: \*Racetrack microtrons, \*Beam steering, Linear accelerators, Electron accelerators, Electron beams, MeV range 10-100, Design, Reprints.

In the NBS-Los Alamos racetrack microtron (RTM), the 17 MeV electron beam, which has made one pass through the RTM linac, is deflected 180 deg in one end magnet and is returned to the same end of the (standing wave) linac for a second pass. A pair of dipole magnets on the linac axis compensate for the beam displacement caused by the end magnet so that the beam enters the linac on axis. These two magnets are designed to have equal field integrals in order to produce a pure displacement. Matching the field integrals was complicated by the quite different widths of the two magnets which have different beam clearance requirements. In addition, the wider magnet contains a quadrupole coil for beam steering. Design considerations are presented. Magnetic field measurements show that critical design goals have been achieved.

101,643 PB91-175521 Not available NTIS National Bureau of Standards (IMSE), Gaithersburg, MD. Reactor Radiation Div.

Fe-W Supermirrors for Polarizing Neutrons.

Final rept.
C. F. Majkrzak, D. A. Neumann, J. R. D. Copley, and R. P. DiNardo. 1988, 6p
Pub. in Proceedings of 1987 Fall MRS Meeting, v103

p115-120 1988.

Keywords: \*Polarizers, Polarization(Spin alignment), Metal films, Thin films, Substrates, Tungsten, Glass, Iron, Sputtering, Reprints, \*Neutron polarizers, \*Supermirrors, Multilayers.

Thin film bilayers of ferromagnetic Fe and nonmagnetic W have been deposited by sputtering on flat glass substrates according to a sequence of gradually vary-ing bilayer thicknesses which in effect extends the critical angle for external mirror reflection for neutrons of one spin state when the Fe is magnetized in the plane of the film. The measured reflectivity of the Fe-W multilayer system is compared with that of other supermirror polarizers consisting of different materials and layer sequences.

101,644 PB91-175547 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Ionizing Radiation Div. Calculation of Beta-Particle Counting Efficiency for Liquid Scintillation Systems with Three Phototubes.

Final rept. A. G. Malonda, and B. M. Coursey. 1988, 6p Pub. in Applied Radiation and Isotopes - International Jnl. of Radiation Applications and Instrumentation 39, n12 p1191-1196 1988.

Keywords: \*Scintillation counters, \*Liquid scintillators, \*Beta detection, Phototubes, Counting, Efficiency, Computation, Reprints.

Formulae are derived for the computation of beta-particle counting efficiency for three-phototube liquid-scintillation counters. It is shown that the counting efficiency for triple coincidences may be computed by considering either the pulse-production probabilities or the non-detection probabilities. Effects due to asymmetry of the phototubes are also evaluated.

101,645 PB91-175588 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Atomic and Plasma Radiation Div. Working Group 2: Atomic Transition Probabilities.

Final rept. W. L. Wiese, 1988, 7p Pub. in Reports of Astronomy, vXXA p117-123 1988.

Keywords: \*Electron transitions, \*Transition probabilities, Oscillator strengths, Literature surveys, Reprints.

Some new activities on the determination of atomic transition probabilities are briefly described and an exhaustive list of new literature references is given which covers all transition probability data for the three year period August, 1984-August, 1987.

101,646 PB91-187088 PB91-187088 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Atomic and Plasma Radiation Div.

Electric Quadrupole and Magnetic Dipole Transition Probabilities In Potassium Isoelectronic Sequence.

M. A. Ali, and Y. K. Kim. 1988, 6p Sponsored by Department of Energy, Washington, DC. Office of Fusion Energy. Pub. in Physical Review A 38, n8 p3992-3997 1988.

Keywords: \*E2-transitions, \*M1-transitions, Forbidden transitions, Transition probabilities, Multicharged ions, Molybdenum ions, Potassium, Reprints.

Electric quadrupole and magnetic dipole transition probabilities between 3p(6)4s doublet S(1/2) and 3p(6)3d doublet D(3/2), doublet D(5/2) levels for K through Mo(23+) have been calculated in the relativistic Dirac-Fock single configuration approximation. The positions of the (excited) 4s doublet S(1/2) level for Mo(74-) Mo(23-) are profitted along with the fine Mn(7+)-Mo(23+) are predicted along with the fine structure splitting in the ground configuration 3p(6)3d.

101,647 PB91-187211 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Temperature and Pressure Div.

H2O(I)-H2O(III)-H2O(L) Triple Point of Water as a Fixed Pressure Point.

Final rept.

N. Bignell, and V. E. Bean. 1988, 5p Pub. in Metrologia 25, n4 p205-209 1988.

Keywords: \*Pressure measurement, \*Water, Phase diagrams, Triple point, Reprints.

An apparatus to use the H2O(I)-H2O(III)-H2O(L) triple-point as a fixed pressure point is described. A technique to establish the three phases simultaneously in the cell is given. The value of the pressure was measured with a piston gage and was found to be 208.829 + or - 0.025 MPa at the 99.7 percent confidence level.

101,648 PB91-187302 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Quantum Metrology Div. Angular Distribution of Ejected Electrons in Resonant Auger Processes of Ar, Kr, and Xe.

Final rept. T. A. Carlson, D. R. Mullins, C. E. Beall, B. W. Yates, J. W. Taylor, D. W. Lindle, and F. A. Grimm. 1989,

Pub. in Physical Review A: General Physics 39, n3 p1170-1185 1989.

Keywords: \*Argon, \*Krypton, \*Xenon, \*Auger effect, Photoelectron spectroscopy, Autoionization, Angular distribution, Reprints.

Angle-resolved electron spectroscopy with the help of synchrotron radiation has been used to study resonate Auger processes near the core shells of Ar2p, Kr3d and Xe4d. Results for the lowest energy resonances have received special attention: argon (Ar2p(3/2)->4s) at a photon energy of 244.4 eV, krypton (Kr3d(5/2)->6p) at 91.2 eV, and xenon (Xe4d(5/2)->6p) at 65.1 eV. The angular distribution parameters, beta, are evaluated for each of the resolved Auger peaks. Most striking is the occurrence of large negative beta values for some of the higher kinetic energy peaks. The results are most apparent under high electron resolution. The beta values near -1 are justified in terms of the angular-momentum transfer theory, which predicts beta = -1 for parity unfavored transitions. Results on the Auger spectra are also given at lower kinetic energies, for shake-up states, and for higher energy resonances, especially those involving vacancies in the core shells of the lower spin states.

PB91-187310 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Quantum Metrology Group. Unusual Degree of Angular Anisotropy in the Res-

onant Auger Spectrum of Kr. Final rept.

J. A. Carlson, D. R. Mullins, C. E. Beall, B. W. Yates, J. W. Taylor, D. W. Lindle, B. P. Pullen, and F. A. Grimm. 1988, 4p

Pub. in Physical Review Letters 60, n14 p1382-1385

Keywords: \*Krypton, \*Auger effect, Photoemission, Anisotropy, Excitation, Reprints.

The angular distribution parameter, beta, has been measured for the resonant Auger spectra in Kr following 3d->5p excitation. Unusually low values, close to 1, were seen for two bands. From optical spectroscopy data these bands are assigned to the final states 4p(4)(triplet P)5p(quartet P(5/2), quartet P(3/2). Accordinated D(5/2).

PB91-187393 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Quantum Metrology Div. Angular Distributions of Electrons in Resonant Auger Spectra.

Final rept. J. W. Cooper. 1989, 3p

Pub. in Physical Review A 39, n7 p3714-3716, 1 Apr

Keywords: \*Auger electrons, Angular distribution, Auger effect, Argon, Reprints.

Recent measurements have shown that the angular distribution of Auger electrons observed in near threshold resonant excitation with energy resolution adequate to partially resolve the multiplet structure corresponding to final core states exhibited a marked change in the angular distributions as a function of final electron energy. A method of calculating these angular distributions is proposed which extends the formalism developed for treating angular distributions in photoeffect via a separation into parity favored and unfavored components. As an example of the use of the method, calculations are presented for the 2p-4s resonant Auger process in Argon and compared with recent experiments.

101,651 PB91-187401 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Quantum Metrology Div. Polarization and Anisotropy of X-ray Emission from Molecules.

Final rept.

P. L. Cowan. 1990, 14p Pub. in Proceedings of International Conference on X-Ray and Inner-Shell Processes (15th), Knoxville, TN., July 9-13, 1990, p696-709.

Keywords: \*Molecular gases, \*X-rays, Angular distribution, Polarization, Anisotropy, Reprints.

X-ray emission from selectively excited core hole states in molecular gases can exhibit strong polarization and anisotropic angular distributions. These ef-

fects are attributable to the creation of an aligned ensemble of excited molecules within the otherwise ran-domly oriented molecular gas. This alignment can be created because the resonant excitation probability of core hole states can be strongly dependent upon the instantaneous molecular orientation. This effect presents a novel opportunity for studying molecular symmetries and the structure of matter in disordered phases.

101,652 PB91-187443 Not available NTIS

National Inst. of Standards and Technology (NML), Gaithersburg, MD. Quantum Metrology Div. Some Historical Remarks Concerning These Conferences: With Emphasis on the X-ray Component.

Final rept.
R. D. Deslattes. 1990, 10p
Pub. in Proceedings of International Conference on X-ray and Inner-Shell Processes (15th), Knoxville, TN., July 9-13, 1990, p3-12.

Keywords: \*X-rays, Inner-shell excitation, Inner-shell ionization, Synchrotron radiation, Historical aspects, Meetings, Reprints.

The text is an essay dealing with historical aspects of the series o International Conference on X-ray and Inner Shell Physics. It is intended as part of the preface to the Proceedings volume of the year's Conference, X-90. It emphasizes not only the earliest meetings but also one that took place earlier and, though not generally considered part of the present sequence, anticipated much of what has transpired subsequently.

PB91-189597 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Atomic and Plasma Radiation Div.

Quantum Electrodynamic Contributions to Spin Orbit Splitting in the Ground State of Aluminum-Like lons.

Final rept. Y. K. Kim, V. Kaufman, J. Sugar, and M. A. Ali. 1988,

Sponsored by Department of Energy, Washington, DC. Office of Fusion Energy, and Howard Univ., Washington, DC.

Pub. in Jnl. of the Optical Society of America B 5, n10 p2225-2229 1988.

Keywords: Multicharged ions, Quantum electrodynamics, L-S coupling, Ground state, Lamb shift, Cobalt ions, Xenon ions, M shell, Reprints, \*Aluminum-like

It is shown that the inclusion of QED corrections for the M-shell electrons substantially improves the agreement between multiconfiguration Dirac-Fock calculations and experimental values on the spin-orbit splitting in the ground state (3s(2)3p(2P)) of Al-like ions. Recommended values of the spin-orbit splitting are presented for Co(14+) through Xe(41+).

101,654 PB91-189605 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Atomic and Plasma Radiation Div.

Relativistic and Correlation Effects in the 2s3p Configuration of Beryllium-Like Ions.

Final rept. Y. K. Kim, A. W. Weiss, and W. C. Martin. 1988, 10p Sponsored by Department of Energy, Washington, DC. Office of Fusion Energy.

Pub. in Jnl. of the Optical Society of America B 5, n10 p2215-2224 1988.

Keywords: Multicharged ions, Oscillator strengths, Excited states, Relativistic effects, Energy levels, Correlation, Reprints, \*Beryllium-like ions.

Relativistic and correlation effects cause several inversions of the 'triplet' and 'singlet' J=1 levels in the 2s3p configuration of Be-like ions. The authors have studied these effects in the range of atomic number Z = 6 - 54 using both relativistic and nonrelativistic multiconfiguration wave functions. Theoretical predictions of energies of these levels with respect to the 2s(2) singlet S(0) ground level are compared with experimental data, and the authors conclude that overall, the predictions for the ions having Z = or > 12 are probably more accurate than the available measurements. Calculated oscillator strengths for these resonance transitions are also reported. Near cadmium (Z = 48), the authors confirm still another inversion due to the complete dominance of relativistic effects, which has been reported earlier in the literature.

101.655 PB91-189746 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Electricity Div.

Observation of Atoms Laser-Cooled Below the Doppler Limit. Final rept.

P. D. Lett, R. N. Watts, C. I. Westbrook, W. D. Phillips, and P. L. Gould. 1988, 4p Sponsored by Office of Naval Research, Arlington, VA.

Pub. in Physical Review Letters 61, n2 p169-172, 11

Keywords: Temperature measurement, Cryogenics, Reprints, \*Ultracold atoms, Sodium atoms, Laser cool-

The authors have measured the temperature of a gas of sodium atoms in 'optical molasses' to be as low as 43 + or - 20 (micro)K. Surprisingly, this strongly vio-lates the generally accepted theory of Doppler cooling which predicts a limit of 240 (micro)K. Several comple-mentary measurements of the ballistic motion of atoms released from the molasses were used to determine the temperature.

101.656 PB91-189753 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Quantum Metrology Div. Doppler Shift Attenuation Lifetime Measurements in (54)Cr Following Thermal Neutron Capture. Final rept.

K. P. Lieb, H. G. Borner, M. S. Dewey, J. Jolie, S. J. Robinson, S. Ulbig, and C. Winter. 1988, 5p Pub. in Physics Letters B 215, n1 p50-54, 8 Dec 88.

Keywords: \*Chromium 54, Interacting boson model, Neutron capture, Thermal neutrons, Doppler broadening, Lifetime, Reprints,

The double crystal spectrometer GAMS4 in combination with the ILL high flux reactor has been used to determine the lifetimes of the 3074 keV (2 sub 3, sup +) and 3720 keV (1,2)+ states in (54)Cr. The initial recoil energy of about 0.5 keV imparted by the primary gamma-radiation after thermal neutron capture in (53)Cr produces Doppler broadened line shapes of the secondary transitions. The large (2 sub 3, sup +)(2 sub 1, sup +) M1 strength of B(M1) = 0.39(6) (mu sub n) squared suggests the (2 sub 3, sup +) state to be of mixed symmetry within the Interacting Boson model

PB91-190009 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Atomic and Plasma Radiation Div. Dielectronic Recombination Rate Coefficients of O(5+) and O(2+).

Final rept. L. J. Roszman. 1989, 3p

Pub. in Physica Scripta T28, p36-38 1989.

Keywords: \*Oxygen ions, Multicharged ions, L-S coupling, Autoionization, Reprints, Dielectronic recombi-

The dielectronic recombination rate coefficients for O(5+) and O(2+) in a single-configuration and LS-coupled atomic model are presented. A model calculation for the effects of thermal equilibration of the final states with the plasma electrons is presented and examined.

101.658 PB91-190033 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Radiation Physics Div. Energy Levels and Transition Probabilities in the

Ground State Configuration of Sulfur-Like Ions. Final rept.

E. B. Saloman, and Y. K. Kim. 1989, 18p Pub. in Atomic Data and Nuclear Data Tables 41, n2 p339-356 1989.

Keywords: \*Energy levels, Forbidden transitions, Multicharged ions, Transition probabilities, Ground state, Reprints, \*Sulfur-like ions.

Theoretical energy levels have been calculated for the terms of the ground state configuration of all the sulfur-like ions of atomic number Z=16-92. Transition probabilities have been obtained for the M1 and E2 transitions are supported by the M2 and E2 transitions. tions within the configuration. The calculations were by

means of a multiconfiguration-Dirac-Fock technique which included perturbatively the Breit interaction and the Lamb shift for the K-, L-, and M-shell electrons. Results are presented which use experimental and semi-empirical fits to the term energies for ions with atomic numbers up to Z = 42. Above Z = 42, purely theoretical results are given. It is shown that the agree-ment between the authors' theoretical results and the semi-empirical values of the term energies improves rapidly as Z increases, with all values in excellent agreement by Z = 42.

101,659

PB91-192567 Not available NTIS Institute of Physics, Belgrade (Yugoslavia).

Experimental Stark Widths and Shifts for Spectral Lines of Neutral and Ionized Atoms: A Critical Review of Selected Data for the Period 1983 through 1988. Bimonthly rept.

N. Konjevic, and W. L. Wiese, c1990, 79p

ington, DC. 20036-9976.

Prepared in cooperation with National Inst. of Standards and Technology, Gaithersburg, MD.
Included in Jnl. of Physical and Chemical Reference
Data, v19 n6 p1307-1386 Nov/Dec 90. Available from American Chemical Society, 1155 16th St., NW, Wash-

Keywords: \*Line spectra, \*Stark effect, Neutral atoms, Positive ions, Line width, Line broadening, Spectral shift, Reviews, Tables(Data).

A critical review of the available experimental data on Stark widths and shifts for spectral lines of non-hydrogenic neutral atoms and positive ions has been carried out. The review covers the period from 1983 through the end of 1988 and represents a continuation of earlier critical reviews up to 1982. Data tables containing the selected experimental Stark broadening parameters are presented with estimated accuracies. Guidelines for the accuracy estimates have been developed during the previous reviews and are summarized. data are arranged according to elements and spectra, and these are presented in alphabetical and numerical order, respectively. Comparisons with comprehensive calculations based either on the semiclassical theory, or--for multiply ionized atoms--on the modified se-miempirical approximation, are made whenever possible, since the comparison with theory has often been a principal motivation for the experiments.

101,660

PC A04/MF A01 PB91-194399 National Inst. of Standards and Technology, Gaithersbura, MD. Stopping Power of Fast Charged Particles in

Heavy Elements. H. Bichsel. Apr 91, 74p NISTIR-4550

Prepared in cooperation with Bichsel (Hans), Seattle,

Keywords: \*Stopping power, Proton bombardment, Charged particles, Excitation, Bethe-Bloch theory.

The stopping power formula from Bethe's theory contains terms which are known only approximately and must be estimated with the use of experimental data. These terms include a material constant, the mean excitation energy of the medium, and the shell-, Blochand Barkas-corrections. In an analysis of measured proton and alpha-particle stopping powers and ranges, modifying parameters have been introduced into these corrections, and the mean excitation energy was simultaneously adjusted, so as to get the closest possi-ble agreement with experimental results. Such an analysis is reported here for elements with atomic numbers  $Z=\sigma r>57$ . The modification parameters introduced for the shell corrections have a simple relation to atomic energy levels. The Bethe theory with the adopted mean excitation energies and proposed adjustments of the shell- and Burkas- corrections predicts stopping powers that are in close agreement with experimental values, within the experimental uncertainties. This agreement was obtained for protons with kinetic energies above about 0.5 MeV, and for heavier ions of charge z at energies above (z - 1.5) MeV/u.

101.661

PB91-194407 PC A03/MF A01 National Inst. of Standards and Technology, Gaithersburg, MD.

#### General

Model for the Non-Perturbative QCD (Quantum

Chromodynamics) Vacuum. M. Danos, D. Gogny, and D. Iracane. Apr 91, 34p NISTIR-4555

Prepared in cooperation with CEA Centre d'Etudes de Bruyeres-le-Chatel, Montrouge (France).

Keywords: \*Quantum chromodynamics, states, Meissner-Ochsenfeld effect, Bose-Einstein condensation, Lagrangian functions, Quarks, Gluons.

By treating the high-momentum gluon and the quark sector as an in principle calculabe effective Lagran-gian, the authors obtain a non-perturbative vacuum state for QCD as an infrared quark-gluon condensate. This vacuum is removed from the perturbative vacuum by an energy gap and supports a Meissner-Ochsenfeld effect. It is unstable below a minimum size and it also suggests the existence of a universal hadronization time. This vacuum thus exhibits all the properties required for color confinement.

101,662

PB91-194423 PC A04/MF A01 National Inst. of Standards and Technology (NML), Gaithersburg, MD. Electron and Optical Physics Div. Technical Activities 1990, Electron and Optical

Physics Division.
C. W. Clark. May 91, 72p NISTIR-4553
See also report for 1989, PB90-207267.

Keywords: \*Research, Far ultraviolet radiation, Soft x rays, Synchrotron radiation, SURF II storage ring, Multi-photon processes, Scanning tunneling microscopy, Electronation collisions, Atomic physics, Radiometry, Calibration, Magnetic films.

The report summarizes technical activities of the NIST Electron and Optical Physics Division during Fiscal Year 1990. These fall into five general areas: soft x-ray radiometry, operation of the SURF-II synchrotron storage ring; electron microscopy and basic surface physics; soft x-ray emission studies; and multiphoton processes. A listing is given of calibration services, publica-tions, talks, and other relevant activities of the Division's staff.

101,663 PB91-194886 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Electricity Div.

Prospects for Electromagnetic Manipulation and Trapping of Antihydrogen.

P. D. Lett, P. L. Gould, and W. D. Phillips, 1988, 14p Pub. in Hyperfine Interactions 44, n1-4 p335-348 1988.

Keywords: \*Antimatter, Storage, Reprints, \*Antihydrogen, \*Atom traps, Laser cooling.

The storage and handling of atomic antimatter pre-The storage and handling of atomic antimatter presents special problems because contact with the walls of any material container is prohibited. Laser cooling and trapping and magnetic trapping techniques for neutral atoms are therefore especially appealing. Here the authors review the basic principles of electromagnetic trapping and laser cooling for neutral atoms, and briefly describe a number of already-demonstrated laser and magnetic traps. They discuss limits on the temperatures achievable by laser cooling, as well as some special problems in the laser cooling of hydrogen/antihydrogen. In particular, they present some gen/antihydrogen. In particular, they present some new results for the case of pulsed cooling.

101.664

PB91-194910 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Quantum Metrology Div. Photoionization Studies of Atoms and Molecules Using Synchrotron Radiation.

Final rept.

D. W. Lindle, 1989, 6p Pub. in Nuclear Instruments and Methods in Physics Research 280, n2-3 p161-166, 10 Aug 89.

Keywords: \*Photoionization, X ray fluorescence, Synchrotron radiation, Reprints.

Photoionization studies of free atoms and molecules have undergone considerable development in the past decade, in large part due to the use of synchrotron radiation. The tunability of synchrotron radiation has permitted the study of photoionization processes near valence- and core-level ionization thresholds for atoms and molecules throughout the Periodic Table. A general illustration of these types of study will be presented,

with emphasis on a few of the more promising new directions in atomic and molecular physics being pursued with synchrotron radiation.

101.665

PB91-194928 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Quantum Metrology Group. Angle-Resolved Photoemission from the Ar 2p Subshell.

Final rept. D. W. Lindle, L. J. Medhurst, T. A. Ferrett, P. A. Heimann, M. N. Piancastelli, S. H. Liu, D. A. Shirley, T. A. Carlson, P. C. Deshmukh, G. Nasreen, and S. Manson. 1988, 4p

Pub. in Physical Review A 38, n5 p2371-2374, 1 Sep

Keywords: \*Inner-shell ionization, \*Photionization, \*Argon, Synchrotron radiation, Photoemission, X rays, Reprints.

The angular distribution for Ar 2p photoionization has been measured from just above threshold to 400 eV photon energy, and calculated in the same energy range using the relativistic random-phase approxima-tion. The experimental and theoretical results exhibit good agreement, but the present results disagree somewhat with earlier Hartree-Fock (HF) calculations, with the HF values found to be significantly higher in the near-threshold region. Possible reasons for this discrepancy are discussed with relevance to the general understanding of inner-shell photoionization phenomena.

101.666

PB91-195016 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Radiometric Physics Div. Low-Pressure Symmetric Discharge Heat Pipe and

DROGS of Eu. Final rept.

H. Maoqi, L. Ronggen, and C. L. Cromer. 1990, 5p Pub. in Acta Optica Sinica 10, n5 p385-389 May 90.

Keywords: \*Heat pipes, \*Europium, Atomic spectra, Excited states, Metal vapors, Reprints, Double resonance optogalvanic spectroscopy.

The authors describe a new low pressure symmetric discharge heat pipe (LPDP) which may be used to generate high Z low pressure metal vapor sample. The authors have studied the double resonance opto-galvan-ic spectroscopy (DROGS) of Eu atom in different pres-sure with the LPDP. Four new lines of Eu from 17341/ cm excited level and three from 16612/cm are observed for the first time. It is verified that such a new LPDP is suitable for studying highly excited state spectroscopy of high Z metal elements.

PB91-195032 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Precision Engineering Div. Relativistic Probability Amplitudes and State Preparation.

Final rept.

E. Marx. 1989, 3p Pub. in Bell's Theorem, Quantum Theory and Conceptions of the Universe, p127-129 1989.

Keywords: \*Quantum electrodynamics, Klein-Gordon equation, Relativistic effects, Quantum mechanics, Wave functions, Charged particles, Antiparticles, Reprints, Probability amplitudes.

The wave function for a spinless charged particle in an electromagnetic field is decomposed into two probability amplitudes, one for a particle and one for an antiparticle. The particle amplitude is specified at the initial time and the antiparticle amplitude at the final time. Time reflection invariance indicates that the preparation of the antiparticle state at the final time should be carried out by observers composed of antiparticles. A model of elementary particles shows how relativistic quantum mechanics can be used to describe all reactions.

101.668

PB91-195123 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Center for Radiation Research.

Glueballs and Hadron Spectroscopy.

Final rept.

S. Meshkov. 1988, 9p

Pub. in Proceedings of the Conference on the Intersections between Particle and Nuclear Physics (3rd), Rockport, ME., May 14-19, 1988, p796-804 1988.

Keywords: \*Glueballs, Pseudoscaler mesons, Spectroscopy, Tensors, Hadrons, Reprints.

Identifying glueballs is intimately intertwined with the study of meson spectroscopy. In the brief review, recent experimental results are compared with QCD inspired predictions for the masses of the 0(-+), 1(+-For the 0(-+), 1(++) mesons. They agree remarkably well. For the 0(-+) and 1(++) systems, these agreements lead to the posibility of identifying additional states as candidates for exotica. A major mystery is why the (2(++) sub gT) states are not seen in J/psi - 2(-+) gamma phi phi, in view of the fact that the OZI-violating mechanism should be a good way to produce glueballs.

101,669

Not available NTIS PB91-195206 National Inst. of Standards and Technology (NML), Gaithersburg, MD. Ionizing Radiation Div. Intensifying Effect of Metallic Screens on the Sensitivity of X-ray Films at 662 keV.

Final rept. E. Navon, C. E. Dick, and G. Barnea. 1989, 4p Pub. in Jnl. of Applied Physics 65, n7 p2852-2855

Keywords: \*X ray film, \*Radiation effects, \*Electron bombardment, KeV range 100-1000, Foils(Materials), Lead(Metal), Aluminum, Copper, Radiation doses, Comparison, Sensitivity, Reprints, Intensification factors, Metal screens.

The relative photographic effect of electrons originating from 662 keV photons interacting in aluminum, copper and lead foils was measured as a function of the foil thickness. Intensification factors on the sensitivity of KODAK AA x-ray films of up to 5.5, 4.6, and 8.7 were determined for aluminum, copper and lead respectively. The equilibrium thicknesses for back screens were found to be 40, 65 and 110 mg/sq cm respectively. For front screens, the equilibrium thick-nesses is 110 mg/sq cm in all cases. The results were compared with the absorbed dose in the film's emulsions, calculated by Monte Carlo methods and found to agree within 10 percent.

101.670

PB91-195289 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Quantum Metrology Group.

Anomalous Lgamma2,3 X-ray Emission Spectrum

of Xe.

M. Ohno, and R. E. LaVilla. 1988, 5p Pub. in Physical Review A 38, n7 p3479-3483 1988.

Keywords: \*Xenon, \*X ray spectra, Emission spectra, Greens function, Fluorescence, Reprints.

The L(gamma 2,3)(2s(sup -1)-> 4p(sup -1)) x-ray emission spectrum (XES) of gaseous xenon was measured in fluorescence with a high resolution vacuum double crystal spectrometer. The spectrum was also calculated by the Green's function method. The agreement is excellent. It is shown that the spectrum can be interpreted essentially in terms of the spectral function of the 4p hole. The effects of the initial 2s hole state on the final 4p hole state are small. The spectrum shows that the quasi-particle picture of a 4p hole in xenon breaks down due to strong 4p(sup -1) <--> 4d(sup -2) 4(n, epsilon)f super Coster-Kronig processes.

101,671

PB91-195453 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Electricity Div. Observation of Atoms Laser Cooled Below the

Doppler Limit.

W. D. Phillips, C. I. Westbrook, P. D. Lett, R. N. Watts, P. L. Gould, and H. J. Metcalf. 1989, 3p Pub. in At. Phy. 11, p633-635 1989.

Keywords: Reprints, \*Ultracold atoms, Sodium atoms, Laser cooling.

The authors have measured the temperature of a three-dimensional gas of laser cooled Na atoms to be as low as 40 + or - 20 microK. This is in strong disagreement with the expected Doppler-cooling limit of 240 microK.

101,672 PB91-195503

Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Atomic and Plasma Radiation Div. Relativistic Distorted-Wave Cross Sections for Electron-Impact Excitations of Berylliumlike Ions.

W. J. Qian, J. P. Desclaux, and Y. K. Kim. 1989, 9p Pub. in Physical Review A 39, n9 p4509-4517 1989.

Keywords: \*Electron-ion collisions, Electron impact, Relativistic effects, Wave functions, Cross sections, Excitation, Reprints, \*Beryllium-like ions.

Relativistic distorted-wave Born (RDWB) cross sections of Be-like ions for excitations from the ground state, 2s(2) singlet S(0), to the 2s2p triplet P(1) and singlet P(1) state by electron impact are reported for Ne(6+) through U(88+). Multiconfiguration Dirac-Fock (MCDF) wave functions were used to describe the target ion states, and the relativistic continuum wave functions were calculated in the field of (frozen) target ion charge distribution with the configuration-av-erage exchange potential. Cross sections are present-ed in compact fitting formulas that allow interpolations to determine cross sections with high precision for arbitrary Be-like ions (10 = or < Z = or < 92) and arbitrary incident energies (T = or < 20 keV).

101,673 PB91-195511 PB91-195511 Not available NTIS National Inst. of Standards and Technology (PL), Gaithersburg, MD. Atomic Physics Div.

Spectrum and Energy Levels of Seven-Times-Ionized Krypton (Kr VIII) and Resonance Lines of Eight-Times-Ionized Krypton (Kr IX). Final rept.

J. Reader, N. Acquista, and V. Kaufman. 1991, 10p Sponsored by Department of Energy, Washington, DC. Pub. in Jnl. of the Optical Society of America B 8, n3 p538-547 Mar 91.

Keywords: \*Krypton ions, \*Line spectra, \*Energy levels, Extreme ultraviolet radiation, Reprints, Copper-

The spectrum of the copperlike ion Kr VIII was observed with a low-inductance spark and 10.7-m normal- and grazing-incidence spectrographs. A total normal- and grazing-incidence spectrographs. A total of 46 new lines with wavelengths ranging from 115 to 696 A were identified: 18 of the type 3d(10)nl-3d(10)nl', 10 of the type 3d(10)4s-3d(9)4s4p, and 18 of the type 3d(10)4p-3d(9)4p(2). From these lines 37 new energy levels were determined: 14 of the type 3d(10)nl, 10 belonging to 3d(9)4s4p, and 13 to 3d(9)4p(2). New values for all known levels were detend by combining the present results with measure. rived by combining the present results with measurements at longer wavelength by Gallardo et al. (Appl. Opt. 28, 5088 (1989)). The ionization energy was found to be 1014 665 + or - 25/cm (125.802 + or - 0.003 eV). New wavelength measurements were made for the 3d(10)-3d(9)4p, 4f resonance lines of the nickellike ion Kr IX.

101,674 PB91-195602 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Atomic and Plasma Radiation Div. Dielectronic Recombination Rate Coefficients for lons of the Fluorine Isoelectronic Sequence. Final rept.

L. J. Roszman. 1989, 2p Sponsored by Department of Energy, Washington, DC. Office of Fusion Energy.

Pub. in Physical Review A 39, n2 p913-914 1989.

Keywords: Isoelectronic sequence, Krypton ions, Molybdenum ions, Selenium ions, Reprints, \*Fluorine-like ions, \*Dielectronic recombination.

The dielectronic-recombination rate coefficients for the fluorine isoelectronic sequence have been revised due to an error for the rate coefficients of Kr(27+) and Mo(33+). Additionally, the calculations of the dielectronic-recombination rate coefficients associated with the delta n = 0 radiative transitions have been extended to include orbital angular momentum values for the Rydberg and continuum electrons as high as 15 and 17 respectively. A separate calculation has been made for the rate coefficient of Se(24+) in order that

comparisons can be made with recently completed relativistic calculations.

PB91-195610 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Atomic and Plasma Radiation Div. Influence of Metastable States and Thermal Equilibration upon Dielectronic Recombination in Low Density to Moderate Density. Final rept.

L. J. Roszman. 1989, 5p Sponsored by Department of Energy, Washington, DC. Office of Fusion Energy. Pub. in Physical Review A 39, n4 p2073-2077 1989.

Keywords: Isoelectronic sequence, Metastable state, Excited states, Reprints, \*Oxygen-like ions, Dielectronic recombination.

The decrease of the dielectronic recombination rate coefficient by the equilibration of the highly excited final states of the process with the plasma continuum is examined for the oxygen isoelectronic sequence. The enhancement of the effective rate of dielectronic recombination by the presence of metastable states in the ground configuration of the initial ion is analyzed for Fe(18+).

101,676 PB91-200816

Not available NTIS National Inst. of Standards and Technology (PL),

Gaithersburg, MD. Atomic Physics Div. 5s(2)5p(2) - (5s(2)5p5d +5s5p(3) + 5s(2)5p6s + 5s(2)5p7s) Transitions in Sb II and 5s(2)5p -(5s5p(2) + 5s(2)nl) Transitions in Sb III. Final rept.

B. Arcimowicz, Y. N. Joshi, and V. Kaufman. 1989,

Pub. in Canadian Jnl. of Physics 67, n6 p572-578 1989.

Keywords: \*Antimony ions, \*Ultraviolet spectra, Electron transitions, Ground state, Reprints.

The spectrum of antimony was photographed in the 575-2300 A region using a hollow cathode and a triggered spark source. The analysis of the 5s(2)5p(2) - (5s(2)5p5d + 5s5p(3) + 5s(2)5p6s + 5s(2)5p7s) transitions in Sb II spectrum was revised and interpreted on the basis of multiconfiguration interaction calculations. Accurate wavelength measurements of Sb III lines lead to a revised ground-state 5s(2)5p doublet P interval value of 6574.5/cm.

101,677 PB91-200840 Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Time and Frequency Div. Clocks, Atomic and Molecular,

Final rept.

J. A. Barnes, and J. J. Bollinger. 1991, 2p See also PB81-236606.

Pub. in Encyclopedia of Physics, p154-155 1991.

Keywords: \*Frequency standards, \*Atomic clocks, Ion traps(Instrumentation), Cesium, Time, Reprints, Laser

Atomic and molecular clocks are described in simple terms using the cesium atomic clock as an example. Some applications of atomic clocks are listed. Current research on frequency metrology including ion traps, laser cooling, and optical frequency standards are dis-

101,678 PB91-200857 Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Time and Frequency Div.

Observation of Correlations in Finite, Strongly

Coupled Ion Plasmas.

J. J. Bollinger, S. L. Gilbert, D. J. Heinzen, W. M. Itano, and D. J. Wineland. 1990, 11p Sponsored by Air Force Office of Scientific Research,

Bolling AFB, DC., and Office of Naval Research, Arlington, VA.

Pub. in Proceedings of Yamada Conference (24th) on Strongly Coupled Plasma Physics, Lake Yamanaka, Japan, August 29-September 2, 1989, p177-187 1990.

Keywords: Laser induced fluorescence, Beryllium ions, Reprints, \*Ion plasmas, Penning traps, Laser cooling.

The authors have observed spatial correlations with up to 15,000 Be(1+) ions in a Penning trap with Gamma

> 100. These correlations are strongly affected by the boundary conditions and take the form of concentric shells as predicted by computer simulations. In the paper the authors briefly describe the experimental confinement geometry and the laser cooling of the ions. Experimental techniques for observing the shell structure are described. The relatively large spacings between the ions permit the shells to be directly viewed by imaging the Be(1+) laser-induced fluorescence onto a photon-counting camera. Diagnostic techniques capable of measuring the ion diffusion are then discussed. Qualitative observations of the ion diffusion are compared with theoretical predictions.

101.679

PB91-200881 Not available NTIS
National Inst. of Standards and Technology (NML), Boulder, CO. Quantum Physics Div.

Near-Threshold Vibrational Excitation of H2 by Electron Impact: Resolution of Discrepancies between Experiment and Theory.

Final rept. S. J. Buckman, M. J. Brunger, D. S. Newman, G. Snitchler, S. Alston, D. W. Norcross, M. A. Morrison, B. C. Saha, G. Danby, and W. K. Trail. 1990, 4p See also PB91-101584.

Pub. in Physical Review Letters 65, n26 p3253-3256, 24 Dec 90.

Keywords: \*Electron-molecule collisions, \*Hydrogen, Vibrational states, Excitation, Reprints.

New measurements and calculations of near-threshold (0.5-5.0 eV) e-H2 vibrational-excitation cross sections challenge previous determinations based on transport analysis. Elastic and mu(o)=0->mu=1 cross sections measured in a crossed electron-molecular-beam apparatus agree well with values calculated using a vibrational close-coupling theory with a separable representation of exchange, particularly at energies below 2.0 eV, but are incompatible with cross sections derived via analysis of electron-swarm transport data.

101.680

PB91-202903 Not available NTIS National Inst. of Standards and Technology (NEL), Boulder, CO. Electromagnetic Technology Div Enhanced Flux Creep in Nb-Ti Superconductors After an Increase in Temperature.

Final rept. R. W. Cross, and R. B. Goldfarb. 1991, 2p Sponsored by Department of Energy, Washington, DC. Pub. in Applied Physics Letters 58, n4 p415-416, 28 Jan 91.

Keywords: \*Superconducting super collider, \*Superconducting cables, Superconducting magnets, Temperature dependence, Magnetization, Relaxation, Reprints, Flux creep, Niobium titanium.

The magnetic fields of Superconducting Super Collider (SSC) dipole magnets change with time when the magnets are operated at constant current. The decay of the field is thought to be a consequence of flux creep in the Nb-Ti filaments in the superconducting cables. However, measured magnetic relaxation of small samples of SSC cable as a function of time is unlike the large decays that are observed in the fields of the actual magnets. The authors have made relaxation measurements on sample SSC conductors at 3.5 and 4.0 K after field cycling. The decay at both temperatures was 2.8% in 50 min. However, the relaxation measured after a temperature increase from 3.5 to 4.0 K was 4.8% in 50 min. A likely reason for the greater magnetization decay is that, after an increase in temperature, the Nb-Ti is in a supercritical state, with shielding currents flowing at a density greater than the new critical current density. This causes enhanced flux creep. The authors suggest that a small temperature rise during the operation of SSC magnets may contrib-ute to the unexpectedly large magnetic field decay.

101.681

Not available NTIS PB91-202911 National Inst. of Standards and Technology (NEL), Boulder, CO. Electromagnetic Technology Div.

Hall Probe Magnetometer for SSC Magnet Cables: Effect of Transport Current on Magnetization and Flux Creep.

Final rept. R. W. Cross, and R. B. Goldfarb. 1991, 3p

Sponsored by Department of Energy, Washington, DC.

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#### General

Pub. in IEEE (Institute of Electrical and Electronics Engineers) Transactions on Magnetics 27, n2 p1796-1798 Mar 91.

Keywords: \*Superconducting super collider, \*Superconducting cables, \*Magnetometers, Superconducting magnets, Magnetic hysteresis, Magnetization, Hall effect, AC losses, Reprints, Flux creep.

The authors constructed a Hall probe magnetometer to measure the magnetization hysteresis loops of Su-perconducting Super Collider magnet cables. The in-strument uses two Hall-effect field sensors to measure the applied field H and the magnetic induction B. Magnetization M is calculated from the difference of the two quantities. The Hall probes are centered coaxially in the bore of a superconducting solenoid with the B probe against the sample's broad surface. An alternative probe arrangement, in which M is measured directly, aligns the sample probe parallel to the field. The authors measured M as a function of H and field cycle rate both with and without a dc transport current. Flux creep as a function of current was measured from the dependence of ac loss on the cycling rate and from the decay of magnetization with time. Transport currents up to 20% of the critical current have minimal effect on magnetization and flux creep.

PB91-202929 Not available NTIS National Inst. of Standards and Technology (NEL), PB91-202929 Boulder, CO. Electromagnetic Technology Div. Correlation of Flux States Generated by Optical Switching of a Superconducting Circuit. Final rept.

E. Cunningham, G. S. Park, B. Cabrera, and M. E.

Huber. 1990, 2p Sponsored by Office of Naval Research, Arlington, VA. Pub. in Physica B 165 and 166, p113-114 1990

Keywords: Optical switching, Magnetic flux, Light pulses, Reprints, \*Superconducting switches.

The authors pulse a superconducting microbridge with light, changing the quantum flux state of a superconducting circuit. Long sequences of pulses are used to measure the degree of correlation between succes-sive flux states. In a series of runs, the pulse length was changed over six decades from 6 ns to 10 ms. The correlations fit a simple Fokker-Planck conditional probability model.

101,683

PB91-203067 Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Quantum Physics Div.

Probe for Real-Time Images of Particle Beams and Their Analyses in a Merged-Beams Apparatus. Final rept.

J. L. Forand, C. Timmer, E. Wahlin, B. D. DePaola, G. H. Dunn, D. R. Swenson, and K. Rinn. 1990, 6p Contract DE-Al05-86ER53237

Sponsored by Department of Energy, Washington, DC. Pub. in Review of Scientific Instruments 61, n11 p3372-3377 Nov 90.

\*Probes(Electromagnetic), Keywords: beams, Charged particles, Real time, Density, Re-

The authors have developed a real-time charged particle beam probe which can be used both as a beam diagnostic (beam tuning) and to quantitatively determine the three-dimensional density distribution of a beam. The probe consists of a microchannel plate, an aluminized phosphor screen deposited on a fiber-optic faceplate, a flexible fiber-optic bundle, and a charge injection device (CID) in tandem. Digital or analog video output of the CID is fed into a computer or oscilloscope, respectively, for analysis or observation. The probe can be moved continuously along the beams' paths to obtain 'pictures' of the beam at any desired interval thus giving three-dimensional form factors. Either beam singly or both beams simultaneously may be observed on the monitor facilitating the task of beam adjustment for optimum overlap. The digital beam adjustment for optimum overlap. The digital output is used for quantitative computation of the beam overlaps. The device is linear with beam intensity, but the performance degrades with time due to beam damage of the microchannel plate.

101.684

PB91-203083 Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Quantum Physics Div.

Measurements of Velocity-Changing Collision Ker-

Final rept

K. E. Gibble, and A. C. Gallagher, 1991, 15p

Grant NSF-PHY86-04504 Sponsored by National Science Foundation, Washing-

ton, DC. Pub. in Physical Review A 43, n3 p1366-1380, 1 Feb

Keywords: \*Atomic collisions, Line broadening, Ground state, Rare gases, Rubidium, Reprints, \*Colli-

Measurements of velocity-changing collision (VCC) kernels are obtained using velocity-selective optical pumping. This is the first measurement of the shape of an elastic VCC kernel over the full thermal range of velocity changes. Since ground-state collisions are studied (quintet 5(1/2)) Rb and He, Ne, Ar, Kr, or Xe),very low buffer-gas pressures can be used, and therefore pressure broadening (dephasing collisions) does not obscure the effects of VCC's. The data are deconvolved to eliminate the effects of the natural linewidth and are then extrapolated with respect to buffer-gas pressure to determine the single-collision limit. For small initial velocities, the measured kernels are consistent with a hard-sphere model for large velocity changes, but differ significantly for small velocity changes. The measured VCC kernels for large initial velocities and large velocity changes do not exhibit the agreement with the hard-sphere kernel. This implies that information about the inter-atomic potential can be obtained from a measurement of VCC kernels. The authors also show the inadequacy of the much-used Keilson-Storer kernel (J. Appl. Math. 10, 243 (1952)).

101.685

PB91-203125 Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Quantum Physics Div. Squeezed Quantum States of Relic Gravitons and

Primordial Density Fluctuations.

Final rept. L. P. Grishchuk, and Y. V. Sidorov. 1990, 9p Pub. in Physical Review D 42, n10 p3413-3421, 15 Nov

Keywords: \*Gravitons, Gravitational waves, Particle production, Quantum mechanics, Black holes, Cosmology, Reprints.

The close relationship between the theory of particle creation in external fields and the theory of quantummechanical squeezed states is clarified. It is shown that relic gravitons (and other primordial perturba-tions), created from zero-point quantum fluctuations in the course of cosmological evolution, should now be in strongly squeezed states. The statistical properties of the stochastic collection of relic gravitational waves are investigated. Some other examples of particle creation, and in particular Hawking's process of black-hole evaporation, are considered in the context of the theory of squeezed states.

PB91-203166 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Center for Radiation Research. Polarizability of the Photon.

Final rept.

Keywords: \*Protons, Scattering cross sections, Dispersion relations, Polarization, Reprints.

The relationship between the static polarizability of the proton and the electric and magnetic polarizabilities obtained from low-energy photon scattering is discussed. It is shown that a consistent picture emerges if one associates the static polarizability with the imaginary part of the forward scattering amplitude, and the photon scattering cross section with the real part.

PB91-203216 Not available NTIS National Inst. of Standards and Technology (NEL), Boulder, CO. Electromagnetic Fields Div. Generalization of the Cornu Spiral for Lossy

Media. Final rept

D. A. Hill. 1991, 3p Pub. in Jnl. of Applied Physics 69, n3 p1772-1774, 1

Keywords: \*Fresnel diffraction, Fresnel integrals, Fresnel zones, Complex variables, Lossy media, Half planes, Reprints, Cornu spiral.

The classical problem of Fresnel diffraction by a straightedge is extended to allow for loss in the medium. The loss modifies the usual Cornu spiral solution because the argument of the Fresnel integral becomes complex. For high loss, the contributions of the outer Fresnel zones are highly attenuated.

101,688

Not available NTIS PB91-203240 National Inst. of Standards and Technology (NML),

Rational rist. of Standards and Formody, (1997).

Boulder, CO. Quantum Physics Div.

Asymptotic Expansions of the Kernel Functions for Line Formation with Continuous Absorption.

Final rept.

D. G. Hummer. 1991, 6p Contract NAGW-766, Grant NSF-AST88-02937 Sponsored by National Aeronautics and Space Admin-

Foundation, Washington, DC., and National Science Foundation, Washington, DC. Pub. in Jnl. of Quantitative Spectroscopy and Radiative Transfer 45, n4 p211-216 1991.

Keywords: \*Line spectra, Radiative transfer, Asymptotic series, Analytic functions, Kernel functions, Line broadening, Reprints.

Asymptotic expressions are obtained for the kernel functions Mn2(tau, alpha, beta) and K2n(tau, alpha, beta) appearing in the theory of line formation with complete redistribution over a Voigt profile with damping parameter alpha, in the presence of a source of continuous opacity parameterized by beta. For alpha o, each coefficient in the asymptotic series is expressed as the product of analytic functions of alpha and eta identically = beta(tau) separately. For Doppler broadening, only the leading term can be evaluated analytically.

101.689

PB91-203257 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Ionizing Radiation Div. NIST High-Dose Calibration Services. Final rent

Final rept.

Pub. in Nuclear Instruments and Methods in Physics Research B40-41, pt2 p1173-1177 Apr 89.

Keywords: \*Radiation doses, \*Dosimeters, \*Calibration, Gamma rays, Measurement, Reprints, Traceability, 1975 lity, US NIST.

There is a need for standardization of high-dose measurements used in the radiation processing industry in order to provide measurement assurance and traceability to national standards. NIST provides dosimetry calibration services to this industry. One of these services involves the administering of known absorbed doses of gamma rays to customer-supplied dosi-meters. The dosimeters are packaged to provide ap-propriate electron equilibrium conditions and are irradiated in a standard (60)Co calibration facility; this provides a calibration of the response of that batch of dosimeters. Another service consists of supplying to a customer calibrated transfer dosimeters for irradiation with the customer's in-house radiation source. The irradiated transfer dosimeters are then returned to NIST for analysis and the results reported to the customer, thereby providing a calibration of the dose rate of the customer's source.

101,690

PB91-203307 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Molecular Spectroscopy Div. Notes and Comments on Roundtable Discussion on Laser-Assisted Collisions and Collision-Induced Spectra.

Final rept.
P. S. Julienne, and L. Frommhold. 1989, 7p Pub. in Spectral Line Shapes, p800-806 1989.

Keywords: Collision broadening, Line broadening, Line spectra, Dipole moments, Reprints, \*Laser assisted collisions, \*Collision induced spectra.

It is especially fitting at the conference, which for the first time brings together the communities on line broadening and collision-induced absorption, that the roundtable sessions on laser-assisted collisions and collision-induced spectra be combined into one dis-

cussion. This enables one to point out the very strong similarities between these two fields, both in the types of phenomena treated and in the methodology used to calculate the spectra. Therefore, as a major theme of the discussion, the authors would like to point out the similarities and differences between the two fields.

101,691 PB91-203315 Not available NTIS National Inst. of Standards and Technology (NEL), Boulder, CO. Electromagnetic Fields Div. Estimation of Electromagnetic Fields in Complex Environments.

M. Kanda, and J. Randa. 1991, 6p

Pub. in Proceedings of the International Zurich Symposium and Technical Exhibition on Electromagnetic Compatibility (9th), Zurich, Switzerland, March 12-14, 1991, p337-342.

Keywords: \*Electromagnetic fields, \*Field strength, \*Estimating, Statistical analysis, Finite element \*Estimating, Statistical analysis, Finite element method, Directional measurement, Reprints, National Institute of Standards and Technology.

The problem of measuring and characterizing complicated multiple-source, multiple-frequency electromagnetic environments is becoming more important and more difficult as electrical devices proliferate. The paper reviews three general approaches to the problem which have been investigated at the National Institute of Standards and Technology (NIST). The three approaches are: a statistical treatment of the spatial distribution of electromagnetic field intensities: a nudistribution of electromagnetic field intensities; a numerical computation using a finite-element (or lattice) form of the electromagnetic action functional; and use of a directional probe to scan a volume. All three methods are still in the development stage, but each appears promising.

Not available NTIS PB91-203372 National Bureau of Standards (NEL), Gaithersburg, MD. Statistical Engineering Div. Experimentation and Measurement.

Final rept. H. H. Ku. 1988, 5p See also PB84-233659.

Pub. in Basic Questions in Fatigue: ASTM STP 924, v1 p9-13 1988.

Keywords: \*Experimental design, Statistical analysis, Variability, Planning, Reprints.

The paper reviews a number of statistical concepts and methods that could be helpful to experiments in the planning stage. These include: (1) sharpening the objective of the experiment, (2) avoiding confounding of experimental factors, and (3) providing realistic estimates of variabilities. Two examples are given.

101,693 PB91-203398 PB91-203398 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Ionizing Radiation Div. Cross-Section Measurements in the Intermediate-Energy Standard Neutron Field.

Final rept. G. P. Lamaze, C. M. Eisenhauer, J. A. Grundl, E. D. McGarry, and F. J. Schima. 1988, 4p Pub. in Proceedings of International Conference on Nuclear Data for Science and Technology, Mito, Japan, May 30, 1988, p1033-1036.

Keywords: \*Neutron cross sections, Cobalt 59 target, Gold 197 target, Indium 115 target, Scandium 45 target, Silver 109 target, Sodium 23 target, Neutron reactions, Fast neutrons, Reprints.

Measured and calculated results are reported for the Measured and calculated results are reported for the spectrum-averaged cross sections of the (115)ln(n,n')(115m)ln, (197)Au(n,gamma)(198)Au, (23)Na(n,gamma)(24)Na, (59)Co(n,gamma)(60)Co, and (45)Sc(n,gamma)(46)Sc reactions in the Intermediate Energy Standard Neutron Field (ISNF) at the National Bureau of Standards (NBS). The ISNF spectrum resembles a fission spectrum at energies above 3.7 MeV; between 0.18 and 3.7 MeV, the spectrum is dominated by neutrons returning from the graphite after several collisions; and at lower energies the shape is determined by the 1/V absorption in the (10). shape is determined by the 1/v absorption in the (10)B shell. The median energy is about 0.58 MeV, with 98% of the neutron fluence rate occuring between 1,2 keV and 5.6 MeV. The fluence was determined by a fluence transfer reaction ((235)U(n,t)(140)Ba) from a well-calibrated (252)Cf fission source.

101 694 PB91-203406 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Ionizing Radiation Div.

Spectrum-Averaged Cross-Section Measurement

of (103)Rh(n,n)(103m)Rh in the (252)Cf Fission Neutron Spectrum.

Final rept.

560 1989.

O. P. Lamaze, F. J. Schima, C. M. Eisenhauer, and V. Spiegel. 1988, 5p Pub. in Nuclear Science and Engineering 100, n1 p43-

47 Sep 88.

Keywords: \*Rhodium 103 target, \*Neutron cross sections, Neutron scattering, Fission neutrons, Inelastic scattering, Dosimetry, Californium 252, Reprints.

Because of the close correspondence of the (103)Rh(n,n') differential cross section and the kerma muscle response function for neutrons, rhodium is an attractive neutron kerma monitor. In support of its use as a neutron monitor, the spectrum averaged cross section, sigma(bar), has been measured for a (252)Cf fission neutron spectrum. Pairs of rhodium foils were irradiated on opposite sides of a thinly-encapsulated (252)Cf neutron source. The neutron fluence incident on the foils is determined by the source strength, average foil distance, and length of time of the irradiation. Corrections are made for neutron scattering, satura-tion of activity, and attenuation of the x-rays in the foil during counting. The x-rays were detected with an intrinsic germanium x-ray detector. The results of five separate irradiations yield a value of sigma(bar)(star)P(Kx)=62.3 + or - 19mb, A dscussions of systematic uncertainties is given.

PB91-203422 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Precision Engineering Div.

Calibration of the NBS 10mum Space Beads. Final rept.

T. R. Lettieri, A. W. Hartman, G. G. Hembree, and E. Marx. 1989, 11p Pub. in Jnl. of Colloid Interface Science 131, n2 p550-

Keywords: \*Microspheres, \*Dimensional measurement, Electron microscopy, Light scattering, Particle size, Diameters, Calibration, Certification, Reprints, Standard reference materials, Space beads, Micro-

A summary is presented of the procedures used to certify NBS Standard Reference Material 1960, nominal 10 micrometer 'space beads'. Three independent micrometrology techniques were used, with the results agreeing to about 0.1%. Center distance finding, a method based on optical microscopy, gave a value of 9.89 + or - 0.04 micrometers which was chosen as the certified mean diameter. Two supporting measurements, made using metrology electron microscopy and resonance light scattering, yielded mean diameters of 9.886 + or - 0.029 micrometers and 9.898 + or -9.000 + 07 - 0.029 micrometers and 9.898 + 07 - 0.029 micrometers, respectively. The main peak of the size distribution for this material is nearly Gaussian, with a certified standard deviation of 0.09 micrometrs, excluding outlying particles. The SRM 1960 microsspace shuttle 'Challenger', making the material the first commercial product to be made in space.

101.696 PB91-203430 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Precision Engineering Div. Dimensional Calibration of an NBS 0.3-mum-Diameter Particle-Sizing Standard. Final rept.

T. R. Lettieri, and G. G. Hembree. 1989, 7p Pub. in Jnl. of Colloid Interface Science 127, n2 p566-572 1989.

Keywords: \*Microspheres, \*Dimensional measurement, Transmission electron microscopy, Light scattering, Particle size, Calibration, Certification, Diameters, Reprints, \*Standard reference materials, Micrometrology.

The article summarizes the procedures used at the National Bureau of Standards (NBS) in the certification of a new submicrometer particle-sizing Standard Refer-ence Material (SRM 1691). The mean diameter of the polystyrene microspheres was accurately measured using two independent micrometrology techniques.

One technique, transmission electron microscopy, measured the particles dried and in a vacuum, and gave a result of 0.269 + or - 0.007 micrometer for the certified mean diameter. The supporting method, quasi-elastic light scattering, yielded a value of 0.276 + or - 0.007 micrometer for the diameter of the microspheres in liquid suspension. Descriptions of the experimental techniques, data analyses, and sources of error are discussed in the paper. The calibrated microspheres are now available from NBS for use as a primary length standard in the submicrometer size range. Applications include microcontamination measurement in semiconductor processing, atmospheric sampling, and electron-microscope calibration.

101,697

PB91-203455 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Office of Standard Reference Data Critical Data in Physics and Chemistry.

Final rept.

D. R. Lide, and B. B. Molino. 1987, 12p Pub. in Encyclopedia of Physical Science and Technology, v3 p786-797 1987.

Keywords: \*Physical properties, \*Chemical properties, Atomic weights, Fundamental constants, Thermodynamics, Fluids, Historical aspects, Reprints, Critical data.

The history and current status of activities related to critical evaluations of physical and chemical data are summarized. A general description of methods for evaluating data is given. Representative tables of important physical and chemical constants are included.

101,698

PB91-203638 Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Quantum Physics Div. Observation of the Cesium Clock Transition Using Laser-Cooled Atoms in a Vapor Cell.

Final rept.

C. Monroe, H. Robinson, and C. Wieman. 1991, 3p. Pub. in Optics Letters 16, n1 p50-52, 1 Jan 91.

Keywords: \*Atomic clocks, Electron transitions, Cesium, Reprints, Atom traps, Laser cooling.

Cesium atoms in a vapor cell have been trapped and cooled by using light from laser diodes. The 6S F = 4, m = 0 -> 6S F = 3, m = 0 hyperfine clock transition was excited as these atoms then fell 2.5 cm in darkness. The authors observed a linewidth of 8 Hz with good signal-to-noise ratio. This gave a short-term fractional frequency resolution of 6.5 x 10 to the -12 power/sec (sup 1/2), and there is potential for substantial improvement. The apparatus is extremely simple and compact, consisting of a small cesium vapor cell and two diode lasers.

101.699

PB91-203778 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Radiation Physics Div. High Harmonic Generation in Hydrogenic Ions. Final rept.

L. Pan, K. T. Taylor, and C. W. Clark. 1989, 4p Pub. in Physical Review A 39, n9 p4894-4897, 1 May

Keywords: \*Harmonic generation, Multi-photon processes, Nonlinear optics, Reprints, \*Hydrogen-like ions, 'Hydrogenic ions.

The authors have calculated the frequency-dependent nonlinear susceptibilities of hydrogenic ions up to very high order of nonlinearity. The critical driving intensity, at which the radiated harmonic intensity of the (q+2)th order, produced by the direct process, exceeds that of the qth order, is found to decrease rapidly with q. The computed values of critical intensity are comparable to those at which 'plateau' behavior is observed in recent experiments.

101,700

PB91-203828 Not available NTIS National Inst. of Standards and Technology (NEL), Boulder, CO. Electromagnetic Technology Div

#### General

Effect of Mechanical Deformation on Nb-Ti Filament Proximity-Effect Coupling at the Edges of SSC Cables.

Final rept.
T. W. Petersen, and R. B. Goldfarb. 1991, 2p Sponsored by Department of Energy, Washington, DC. Div. of High Energy Physics.

Pub. in IEEE (Institute of Electrical and Electronics Engineers) Transactions on Magnetics 27, n2 p1809-1810 Mar 91.

Keywords: \*Superconducting super collider, \*Superconducting cables, Superconducting magnets, Magnetic fields, Proximity effect, Time dependence, Magnetic fields, Proximity effect, Proxim netization, Deformation, Reprints, Niobium titanium.

Magnetization as a function of transverse magnetic field and time was measured for short strands extracted from the centers and edges of five Nb-Ti Rutherford cables designed for use in Superconducting Super Collider dipole magnets. The multifilamentary strands all had 6-micrometer diameter filaments. Edge samples, which had severe mechanical deformation, showed small magnetic coupling losses at low fields, compared to no coupling losses for undeformed center strands. Sharp strand bends at cable edges decreases the interfilament spacing to the order of the coherence length in the normal matrix material which increases the effective filament diameter and hysteresis loss at low fields. Microscopic studies of the cables' cross sections confirmed smaller interfilament separations in these samples. Flux creep measurements, represented by the time dependence of magnetization, showed little difference between edge and center samples. This indicates that the proximity-coupled matrix in edge samples is not a significant source of flux creep.

101,701 PB91-203919

Not available NTIS
National Inst. of Standards and Technology (NEL),
Boulder, CO. Electromagnetic Technology Div.
New Look at the Bitter Method of Magnetic Imaging. ing.

Final rept.
P. Rice, and J. Moreland. 1991, 2p
Pub. in Review of Scientific Instruments 62, n3 p844-

Keywords: Scanning tunneling microscopy, Magnetic storage, Magnetic disks, High resolution, Imaging techniques, Ferrofluids, Reprints, \*Bitter method, \*Magnetic imaging.

A scanning tunneling microscope (STM) was used in place of an optical microscope in the Bitter method to image the magnetic ferrofluid particles on the surface of a hard disk. The resolution obtainable with the usual Bitter method is limited by the optical viewing of the magnetic particles. Using the scanning tunneling microscope, the output place and particles are resolved. croscope, the authors have obtained image resolution limited only by the ferrofluid particle size.

101.702 PB91-204115 Not available NTIS Not available NTIS
National Inst. of Standards and Technology (NML),
Boulder, CO. Quantum Physics Div.
Test of the Inverse-Square Law of Gravitation
Using the 300-m Tower at Erie, Colorado.

Final rept.
C. C. Speake, T. M. Niebauer, M. P. McHugh, P. T.
Keyser, J. E. Faller, J. Y. Cruz, J. C. Harrison, J.
Makinen, and R. B. Beruff, 1990, 5p
Pub. in Physical Review Letters 65, n16 p1967-1971,

15 Oct 90.

Keywords: \*Gravitation, Basic interactions, Towers, Tests, Reprints, Inverse square laws, Fifth force.

Gravity was measured at eight different heights on a 300-m meteorological tower using LaCoste and Romberg gravimeters. The observed values were adjusted for tides, drift, and gravimeter screw errors, and tested for systematic effects due to tower motion. These results are compared with values predicted using New-ton's inverse-square law from surface gravity. The dif-ferences exhibit no systematic trends and their rms value is well within the estimated errors of the experiment. This result places new constraints on the possible strength and range of any non-Newtonian force.

PB91-204164 Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Quantum Physics Div.

Collisional Energy Transfer between Excited Sr

Atoms.
Final rept.
H. G. C. Werij, M. Harris, J. Cooper, A. Gallagher, and J. F. Kelly. 1991, 13p
Contract NSF-PHY86-04504

Sponsored by National Science Foundation, Washington, DC.

Pub. in Physical Review A 43, n5 p2237-2249, 1 Mar

Keywords: \*Atomic collisions, \*Strontium, Excited states, Reprints, Collisional energy transfer.

The following energy-transfer reactions have been ob-The following energy-transfer reactions have been observed in a Sr vapor following pulsed excitation of the 5 singlet P(1) state. The r singlet D(2) state was populated by a nonlinear stimulated process. By measuring the rate coefficients for these reactions for over 40 final states n(sup (2s + 1))L, one looks for insight into how these reactions depend on energy defect, spin, and angular momentum. It is found that there is not a very strong dependence on the energy defect and avery strong dependence on the energy defect, and that singlet and triplet final states are produced in comparable amounts. The final states tend to be populated more effectively as their angular momentum increases. Total rate coefficients are of the order of gaskinetic rates.

101,704 PB91-216705 PC A07/MF A02 National Inst. of Standards and Technology, Gaithers-

burg, MD.
Journal of Research of the National Institute of Standards and Technology. May-June 1991. Volume 96. Number 3. 1991, 150p

Also available from Supt. of Docs. as SN703-027-00040-7. See also PB91-216713 through PB91-216762 and PB91-187617. Library of Congress catalog card no. 89-656121.

Keywords: \*Research, Thermal conductivity, Thermal diffusity, Fluids, Surface roughness, Quality control, Nondestructive tests, Transistors, Crystal growth, Crystal defects, Time series analysis, Signal processing, Acoustic emissions, Second breakdown.

Contents:

A High-Temperature Transient Hot-Wire Thermal Conductivity Apparatus for Fluids; Standard Reference Specimens in Quality Control

of Engineering Surfaces; An Automated Reverse-Bias Second-Breakdown Transistor Tester;

High Resolution Synchrotron X-Radiation Diffraction Imaging of Crystals Grown in Microgravity and Closely Related Terrestrial

Root Projection of One-Sided Time Series; Deconvolution of Acoustic Emission and Other Causal Time Series.

101,705 PB91-216812 PC A04/MF A01 National Inst. of Standards and Technology (PL), Gaithersburg, MD.
Evidence for Surface alpha Particle Clusters in

(nat)AG(197)Au from the (e,alpha) Reaction. W. R. Dodge. Jun 91, 57p NISTIR-4495

Keywords: \*Alpha particles, \*Cluster model, \*Gold 197 target, \*Silver, \*Electron reactions, MeV range 100-1000, MeV range 10-100, Electroproduction, Protons, Graphs(Charts).

The (nat) Ag and (197) Au (e,p) and (e, alpha) energy and angular distributions were measured at 6 electron bombarding energies between 50 and 115 MeV at the National Institute of Standards and Technology. The (nat) Ag and (197) Au (e,p) angular distributions exhibit an asymmetric component which increases from 0 to 50% as the proton energy increases from the proton (e, alpha) angular distributions exhibit an asymmetric component which increases from 0 to 30% as the alpha energy increases from the alpha particle Cou-lomb barrier to 26 MeV. The authors conclude that the asymmetric component of the proton and alpha particle yields are the result of direct or semidirect processes rather than resonance processes and hence, be-cause of the short mean free paths of alpha particles in nuclear matter, give evidence for the existence of alpha particle clusters in the nuclear surface.

101,706 PB91-236604

Not available NTIS

National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Reactor Radiation Div.

Transmission Properties of a Counter-Rotating

Pair of Disk Choppers. Final rept.

J. R. D. Copley. 1991, 10p Pub. in Nuclear Instruments and Methods in Physics Research A303, p332-341 1991.

Keywords: \*Neutron choppers, Time-of-flight spectrometers, High resolution, Crosstalk, Design, Reprints.

Counter-rotating pairs of disk choppers are used to provide pulsed neutron beams for thermal neutron scattering experiments. An important advantage of this type of device, compared with the single disk chopper, is that each disk can be equipped with several slots. A choice of slot widths is then made possible, simply by changing the relative phasing of the two disks. The resolution of an instrument with counter-rotating chopper pairs can therefore be altered without having to modify the incident wavelength or the speed of the choppers. A potential problem, when there are several slots in each disk, is that there will be 'cross talk', i.e. neutrons will be transmitted by a pair of slots other than the intended combination. The author examines that the interded combination. The author examines the transmission properties of a counter-rotating pair of choppers, and describes methods to determine whether or not cross talk can occur. An important conclusion is that the axial separation between the two choppers must be included in the analysis; this separa-tion, which is generally small (of order several cm), sig-nificantly increases the potential for unwanted cross talk. The author briefly discusses the implications of cross talk in the design of a high resolution time-offlight spectrometer.

101,707

PB91-236745 Not available NTIS National Inst. of Standards and Technology (PL), Gaithersburg, MD. Electron and Optical Physics Div. Associative Ionization of Ultra-Cold Laser Trapped Sodium Atoms.

Final rept.
P. L. Gould, P. D. Lett, R. N. Watts, C. I. Westbrook, P. S. Julienne, W. D. Phillips, H. R. Thorsheim, and J. Weiner. 1989, 14p
Pub. in At. Phys. 11, p215-228 1989.

Keywords: \*Sodium atoms, Reprints, \*Associative ionization, Ultracold atoms, Laser cooling, Laser trapping.

The authors describe their recent investigations of associative ionization in laser cooled sodium confined in a new type of laser trap. Their measured cross section at a temperature < 1 mK is three orders of magnitude larger than that measured in previous experiments at higher temperatures. The authors have also seen a dramatic influence of laser intensity on the collision dy-

101.708

PB91-236828 Not available NTIS National Inst. of Standards and Technology (PL), Boul-der, CO. Time and Frequency Div. Reply to Comment on 'Quantum Zeno Effect'. Final rept.

Final rept. W. M. Itano, D. J. Heinzen, J. J. Bollinger, and D. J. Wineland, 1991, 2p See also PB90-254715.

Pub. in Physical Review A 43, n9 p5168-5169, 1 May

Keywords: Quantum mechanics, Ion storage, Reprints, \*Quantum Zeno effect, \*Zeno effect, Laser cooling, Penning traps.

Various interpretations of quantum mechanics are valid insofar as they predict the same experimental results. Some invoke 'wave-function collapse' and some do not. An interpretation based on the collapse postulate provides a simple explanation for a recent experimental demonstration of the quantum Zeno effect (Itano et al., Phys. Rev. A-41, 2295 (1990)), but other interpretations are also valid.

101,709

PB91-236976 Not available NTIS National Inst. of Standards and Technology (EEEL), Boulder, CO. Electromagnetic Fields Div.

General

Cryogenic Fatigue of High-Strength Aluminum Alloys and Correlations with Tensile Properties. Final rept.

L. Ma, J. K. Han, R. L. Tobler, R. P. Walsh, and R. P. Reed. 1990, 8p

Sponsored by Department of Energy, Washington, DC. Office of Fusion Energy, and Universities Research Association, Berkeley, CA. Superconducting Super Collider Central Design Group.

Pub. in Advances in Cryogenic Engineering (Materials), 1926–2725, 2921, 1000

als), v36 p375-382 1990.

Keywords: \*Superconducting super collider, \*Aluminum alloys, \*Stress tests, \*Cryogenic storage devices, Tensile strength, Fatigue life, Metal sheets, Reprints, Aluminum alloy 7075, Aluminum alloy 7475, Aluminum alloy 2219, Aluminum alloy 2090.

Notched and unnotched sheet specimens of four alunoticined and unnotched sheet specimens of four aluminum alloys were fatigue tested to evaluate potential use in the Superconducting Super Collider. Alloys 7075-T6, 7475-T761, 2219-T87, and 2090-T8E41 were tested in axial fatigue at a stress ratio of 0.1. The unnotched specimens were tested at 295, 76, and 4 K, whereas notched specimens were tested at 76 K only. The fatigue strengths of these alloys were compared with a practical interest in a life of 100,000 cycles. Fatigue strengths with static tensile strengths for notched and unnotched specimens.

101,710 PB91-237115 Not available NTIS National Inst. of Standards and Technology (EEEL), Gaithersburg, MD. Electricity Div. Monitoring the Mass Standard via the Comparison

of Mechanical to Electrical Power.

Final rept.

P. T. Olsen, W. L. Tew, E. R. Williams, R. E. Elmquist, and H. Sasaki. 1991, 6p See also PB91-101501. Pub. in IEEE (Institute of Electrical and Electronics En-

gineers) Transactions on Instrumentation and Measurement 40, n2 p115-120 Apr 91.

Keywords: \*Mass, \*Standards, Superconducting mag-nets, Rest mass, Hysteresis, Monitoring, Balances, Comparison, Reprints, \*Kilogram, Watt.

The paper presents the current status of the NIST SI watt experiment. Included are goals for the near future as well as projections regarding the viability of monitor-ing and/or replacing the kilogram mass standard. Al-though several significant systematic errors have yet to be evaluated, the standard deviation of the mean of the authors' present measurement distributions is 0.05 ppm.

101,711 PB91-237461 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Gas and Particulate Science Div. Structure of Odd-Odd (132)Sb.

Final rept. C. A. Stone, W. B. Walters, and S. H. Faller. 1989,

9p Pub. in Physical Review C 39, n5 p1963-1971 1989.

Keywords: \*Antimony 132, Nuclear energy levels, Nuclear structure, Fission products, Lifetime, Reprints.

New information is presented on the decay of 40-s (132)Sb. A second beta-fed 1+level was identified in (132)Sb. A second beta-fed 1 + level was identified in Sb; it lies at an energy of 2268 keV and is fed by a relatively strong 0.83% beta-decay branch. Four gamma rays were identified that form a weakly populated cascade from a level at 483 keV. Coincidence data demonstrate that the 254-keV level in this cascade is the 102-ns isomer identified previously by Clark et al. A 96-keV, isomeric gamma ray has also been observed that is placed in the decay of the 4.1-min, 8-isomer in (132)Sb. It may also be the 96-keV transition that is associated with the 1.8 microsec isomer identified in the A=132 chain by Clark et al. The splitting of the levels in the proton-neutron multiplets is discussed the levels in the proton-neutron multiplets is discussed and compared with the results of several recent shell model calculations.

PB91-237495 Not available NTIS National Inst. of Standards and Technology (PL), Gaithersburg, MD. Atomic Physics Div. Extreme-Ultraviolet Spectra of Pd, Ag, Cd, and Sn Ions Observed In a 1.3-keV Tokamak Plasma.

Final rept. J. Sugar, V. Kaufman, and W. L. Rowan. 1991, 4p Sponsored by Department of Energy, Washington, DC. Pub. in Jnl. of the Optical Society of America B 8, n5 p913-916 May 91.

Keywords: \*Plasma spectra, Isoelectronic sequence, Extreme ultraviolet radiation, Ultraviolet spectra, Palladium, Silver, Cadmium, Reprints, Cadmium-like ions, Chlorine-like ions, Potassium-like ions, Sulfur-like ions.

The elements Pd, Ag, Cd, and Sn were each injected by laser ablation into a tokamak plasma of 1.3-keV electron temperature. Spectra in the range of 50-400 A were observed photographically with a 2.2-m grazing-incidence spectrograph. The authors identified lines in the isoelectronic sequences of S, Cl, Ar and K that were not previously classified. They fall in the range of 51-78 A and were measured with an uncertainty of + or - 0.010 A. Graphs of the differences between the measured and the calculated transition energies vary smoothly and confirm the identifications. Least-squares fits to these differences permit accurate pre-dictions for elements Tc, Ru, Rh, and In that have not been investigated. Similar fits to ground-state doublet splittings in the CI and K sequences provide accurate values of magnetic dipole transition energies for these

101,713 PB91-237503 Not available NTIS National Inst. of Standards and Technology (PL), Gaithersburg, MD. Atomic Physics Div. Spectra of the P I Isoelectronic Sequence from Co XIII to Mo XXVIII.

Final rept.
J. Sugar, V. Kaufman, and W. L. Rowan. 1991, 5p
Contract DE-AC05-78ET-53043

Sponsored by Department of Energy, Washington, DC. Pub. in Jnl. of the Optical Society of America B 8, n1 p22-26 Jan 91.

Keywords: \*Plasma spectra, Isoelectronic sequence, M1-transitions, Soft x rays, Reprints, \*Phosphorus-like

Phosphorus like spectra Cu XV to Mo XXVIII have been identified in tokamak- and laser-produced plasmas in the wavelength range of 83 to 163 A. These were obtained with the TEXT tokamak at the University of Texas and the 1-GW Nd:glass laser at the National Institute of Standards and Technology, using 2.2- and 10.7-m grazing-incidence spectrographs, respectively. Wavelength measurements were made with an uncertainty of  $\pm$  or  $\pm$  0.005 A. All the classified lines arise from the 3s(2)3p(3)-3s(2)3p(2)3d array. They were identified through detailed comparisons with Hartree-Fock calculations of wavelengths and relative intensi-ties along the isoelectronic sequence. All spectra from Cu to Mo were observed, except for Rb and Sr, whose Cu to Mo were observed, except for Rb and Sr, whose wavelengths are predicted by interpolation with an uncertainty of + or - 0.02 A. By means of previously observed magnetic-dipole (M1) lines within the 3s(2)3p(3) ground configuration and comparisons with published Dirac-Fock calculations, all the energy levels of the configuration were determined with an uncertainty of + or - 10 to/100 cm for Co to Mo. These levels were used to predict all the M1 wavelengths. A correction to the Co XIV ground configuration is made by means of a previously published list of M1 lines.

101,714 PB91-237511 PB91-237511 Not available NTIS
National Inst. of Standards and Technology (PL),
Gaithersburg, MD. Atomic Physics Div.
Beam-Foil Study of Two-Electron Transitions in

Cu-Like lons. Final rept.

J. Sugar, E. Trabert, G. Moller, P. H. Heckmann, J. H. Blanke, and I. Martinson. 1991, 6p Pub. in Physica Scripta 43, p484-489 1991.

Keywords: Extreme ultraviolet radiation, Ultraviolet lasers, Electron transitions, Niobium ions, Molybdenum ions, Silver ions, Reprints, \*Copper-like ions.

The transition 3d(10)4p doubletP(0)-3d(9)4s(2) dou-The transition 30(10)4p doubletP(0)-30(9)4s(2) doublet D in Cu-like ions, the XUV laser transition proposed by Morley and Sugar, has now been identified in delayed spectra obtained with foil-excited ion beams of Nb, Mo and Ag Calculations of the wavelengths agree closely with the observations, but the observed decay times are significantly larger than the theoretically expected lifetimes. It is shown that the lifetime is probable observed by long lived exceedes from the probably obscured by long-lived cascades from the lowest-lying quartet levels.

PB91-237594

Not available NTIS

National Inst. of Standards and Technology (PL), Gaithersburg, MD. Physics Lab. Office.

Basic Standards and Fundamental Constants.

Final rept.

B. N. Taylor. 1989, 3p
Pub. in IEEE (Institute of Electrical and Electronics Engineers) Transactions on Instrumentation and Measurement 38, n2 p164-166 1989.

Keywords: \*Fundamental constants, \*Electrical measurement, \*Standards, Josephson effect, Least squares method, Reprints, Quantum Hall effect.

These introductory remarks to the panel discussion on Basic Standards and Fundamental Constants at the 1988 Conference on Precision Electromagnetic Measurements (CPEM) touch upon two topics: the importance of precision electromagnetic measurements to the fundamental constants and vice versa; and the idea that recent advances in the determination of a number of constants may have made future leastsquares adjustments of the constants unnecessary.

PB91-237750 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Atomic and Plasma Radiation Div. Spectroscopic Data Base for Carbon and Oxygen.

Final rept. W. L. Wiese. 1989, 2p Pub. in Physica Scripta T28, p10-11 1989.

Keywords: \*Carbon, \*Oxygen, \*Atomic energy levels, \*Transition probabilities, \*Ionization, Spectrum analysis, Wavelengths, Reprints, \*Spectroscopic data.

Comprehensive compilations of critically evaluated spectroscopic data for all stages of ionization of carbon and oxygen are briefly reviewed, especially with respect to their scope and the accuracy of the listed data. The spectroscopic quantities covered are wavelengths, energy levels, and transition probabil-

101,717

PB91-237768 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Atomic and Plasma Radiation Div. Unified Set of Atomic Transition Probabilities for Neutral Argon. Final rept.

W. L. Wiese, J. W. Brault, K. Danzmann, M. Kock, and V. Helbig. 1989, 11p Pub. in Physical Review A 39, n5 p2461-2471 1989.

Keywords: \*Argon, \*Atomic energy levels, \*Transition probabilities, Atomic spectra, Electron transitions, Reprints, \*Atomic transition probabilities, \*Atomic life-

While the atomic transition probabilities and radiative lifetimes of neutral argon have been the subject of numerous experiments and calculations, the results exhibit numerous discrepancies and inconsistencies. The authors present for the first time a unified set of atomic transition probabilities, which is consistent with essentially all recent results, sometimes after critical re-analysis. The data consistency and scale confirmation has been achieved in two ways: (1) The authors have carried out some lifetime/branching ratio measurements for a principal 5p level and the associated 4s-5p transitions. These measurements have very closely confirmed the accuracy of the results of recent independent emission experiments. (2) The authors have critically re-analyzed and revised the literature data for the 4s-4p transitions, as well as utilized the results of a similar critical analysis for the 4s-5p transition array, to establish complete sets of absolute data for these arrays. They have found these data to be mutually consistent from cross-correlation checks between the two arrays using recent literature data. Finally, they have proposed renormalization factors for other argon transitions based on the analysis.

PB91-240762 PC A04/MF A01 National Inst. of Standards and Technology (MSEL), Gaithersburg, MD. Polymers Div. High Magnetic Field Facilities In Japan Related to

Superconductivity Research (Japan Technology

Program). R. D. Shull. Aug 91, 62p NISTIR-4593

Keywords: \*Magnetic fields, \*Superconductors, Research facilities, Superconducting magnets, High tem-

### General

perature superconductors, Critical current, Critical field, Magnetic resonance, Japan, \*Foreign technology, \*High magnetic fields.

The report describes the high magnetic field facilities presently available in Japan and how those facilities are being used for the study of superconducting materials. Particular attention is devoted to Japanese technological advances in the development of superconducting materials which may have an impact on the construction of future high magnetic field facilities. Both pulsed magnetic field facilities and constant field generation are evaluated. In addition, future facilities to become available in Japan are listed.

101,719 PB92-109032 PC A04/MF A01 National Inst. of Standards and Technology (PL), Gaithersburg, MD.
International System of Units (SI).

Special pub. (Final). B. N. Taylor. Aug 91, 64p NIST/SP-330 Also available from Supt. of Docs. as SN003-003-03099-6. Supersedes PB86-244159.

Keywords: \*International system of units, \*Metric system, \*Units of measurement, Primary standards, Translations, \*Foreign technology, International Bureau of Weights and Measures.

The booklet is the United States of America edition of the English-language translation of the sixth edition of Le Systeme International d'Unites (SI), the definitive reference on the SI published in 1991 by the International Bureau of Weights and Measures (BIPM) in the French language. The USA edition conforms in sub-stance with the English-language translation that fol-lows the French-language text in the BIPM publication. That translation was a joint effort of the BIPM, the National Institute of Standards and Technology (NIST) in the United States, and the National Physical Laboratory (NPL) in the United Kingdom. However, to make the booklet helpful to the broadest community of users in the USA, it was necessary to follow current Federal policy, to recognize present USA practices as they are found in the literature of the authors domestic volun-tary standards organizations such as ASTM and IEEE, and to use American spelling of certain words. Thus, the USA edition differs from the English-language version in the BIPM publication in the following details: (1) the dot is used instead of the comma as the decimal the dot is used instead of the comma as the decimal marker; (2) the American spellings 'meter', 'liter', and 'deka' are used instead of 'metre', 'litre', and 'deca'; (3) a small number of footnotes are added for explanatory purposes and to identify USA practices that differ from those suggested in the BIPM publication; (4) in a few instances, American rather than British spelling or usage is followed for a few common words; and (5) the index has been moderately expanded.

PC A04/MF A01 PB92-112358 National Inst. of Standards and Technology (EEEL), Boulder, CO. Electromagnetic Technology Div.

Magnetic Measurements for High Energy Physics Applications. Final rept. Jun 15 88-Jun 14 91. R. B. Goldfarb. Aug 91, 69p NISTIR-3975 Contract DE-AI05-85-ER40240

Sponsored by Department of Energy, Washington, DC. Div. of High Energy Physics.

Keywords: \*Superconducting magnets, \*Superconducting cables, Superconducting wires, Superconducting super collider, High energy physics, Time depend-ence, Magnetic fields, Critical current, Eddy currents, Magnetization, AC losses, Niobium titanium, Flux

The report is a collection of papers describing magnetic measurements on multifilamentary Nb-Ti superconductor wires and cables as a function of magnetic field and time at liquid-helium temperatures. The papers deal with ac losses and interfilament coupling by prox-imity effect and eddy currents. Flux creep was investi-gated under different experimental conditions. A Hallprobe magnetometer, which was used to measure magnetization and flux creep in the presence of a transport current, is described. A method for increasing the critical current of superconducting cable by controlling twist pitch is demonstrated. A critical-state model for the magnetization of superconductors was developed for samples with field-dependent critical current density and rectangular cross section.

101,721 PB92-112481

PC A04/MF A01

National Inst. of Standards and Technology (TS), Gaithersburg, MD. Standards Code and Information

Criteria for the Operation of Federally-Owned Secondary Calibration Laboratories (Ionizing Radiation)

Special pub. (Final). E. H. Eisenhower. Aug 91, 66p NIST/SP-812 Also available from Supt. of Docs. as SN003-003-

Keywords: \*Ionizing radiation, \*Survey monitors, \*Dosimeters, \*Calibration, \*Laboratories, Performance standards, Gamma rays, X rays, Beta particles, Alpha particles, Neutrons, Criteria, Secondary laboratories, Accreditation.

The document contains standards of performance for laboratories that calibrate instrumentation used to measure ionizing radiation. Such standards are useful for the development of a secondary level of calibration laboratories that can provide a high-quality link between the National Institute of Standards and Technology and those who make routine measurements at the field level. The standards may also be used as criteria on which a decision is based regarding accreditation of a particular laboratory. They were developed by representatives of federally-owned laboratories that perform calibrations of the type addressed by the document. The first major part contains general criteria that must be satisfied by all laboratories seeking accreditation. It includes requirements relating to management and staff, physical aspects of the laboratory, calibrations facilities and equipment, operational procedures, accuracy and quality assurance, and records and reports. Five subsequent major parts establish criteria for calibration of survey instruments, irradiation of personnel dosimeters, calibration of sources, calibration of instruments for diagnostic levels, and calibration of reference-class instruments. The types of radiation covered include gamma rays, x rays, beta particles, neutrons, and alpha particles. An appendix describes the proficiency tests administered by NIST to secondary laboratories as a prerequisite for their accredita-

Not available NTIS PR92-116474 National Inst. of Standards and Technology (NML), Boulder, CO. Time and Frequency Div. 303-MHz Frequency Standard Based on Trapped Be(+) lons.

Gilbert, and D. J. Heinzen, W. M. Itano, S. L. Gilbert, and D. J. Wineland. 1991, 3p Sponsored by Office of Naval Research, Arlington, VA., and Air Force Office of Scientific Research, Bolling AFB, DC

Pub. in IEEE (Institute of Electrical and Electronics Engineers) Transactions on Instrumentation and Measurement 40, n2 p126-128 Apr 91.

Keywords: \*Frequency standards, \*Atomic clocks, Hyperfine structure, Beryllium ions, Beryllium 9, Ground state, Ultrahigh frequency, Doppler effect, Reprints, Laser cooling, Penning traps, Ion traps.

A 303-MHz hyperfine transition in the ground state of (9)Be(1+) was used as a basis of a frequency standard. The ions were stored in a Penning ion trap. Linewidths as narrow as 900 micro Hz were obtained. The frequency stability was measured to be better than 3 x 10 to the -12 power/square root of tau. The inaccuracy in the second-order Doppler shift was reduced to 5 parts in 10 to the 15th power by laser cooling. An apparent pressure shift with an unexpectedly large value was discovered which limits the accuracy of the current experiment to approximately 1 part in 10 to the 13 power.

101,723 PB92-116706 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Ionizing Radiation Div.

Dosimetry of a Nearly Monoenergetic 6- to 7-MeV Photon Source by NaI(TI) Scintillation Spectrome-

K. C. Duvall, S. M. Seltzer, C. G. Soares, and B. W. Rust. 1988, 5p

Pub. in Nuclear Instruments and Methods in Physics Research 272, n3 p866-870 Nov 88.

Keywords: \*Gamma dosimetry, \*Nal detectors, Scintillation counters, MeV range 01-10, Radiation protection, Fluorine 19 target, Proton reactions, Spectra unfolding, Calibration, Kerma, Reprints.

The dosimetry of a nearly-monoenergetic 6- to 7-MeV photon source developed at the National Bureau of Standards (NBS) for radiation protection instrument calibration has been carried out by Nal(TI) scintillation spectrometry. The approach uses calculated 3-inch x inch Nal(TI) detector-response functions that been shown to be reasonably accurate up to 20 MeV. A least-squares fit of the appropriate response functions to a selected region of the pulse-height distribution determines the primary 6- to 7-MeV photon fluence. The uncertainty in the fluence determination is based on the chi squared of the fit, the statistics of the data, and the uncertainty in the response functions. The air kerma delivery due to the primary photons at a reference point in the photon field is calculated from the primary photon fluence.

101,724

PB92-116714 Not available NTIS National Bureau of Standards (NML), Gaithersburg, MD. Atomic and Plasma Radiation Div.

Atomic Spectroscopy in the 20th Century - A Tribute to Sitterly, Charlotte Moore, on the Occasion of Her 90th Birthday. Final rept.

B. Edlen, and W. C. Martin. 1988, 4p Pub. in Jnl. of the Optical Society of America B 5, n10 p2039-2042 1988.

Keywords: \*Atomic spectroscopy, Reprints, Sitterly Charlotte Moore.

The introduction describes several areas of atomic spectroscopy represented by 24 papers to be published in a feature issue of J. Opt. Soc. Am. B. This feature issue i a tribute to Charlotte Moore Sitterly on the ocassion of her 90th birthday. The introductory material includes an appreciation of Dr. Sitterly's career at

101.725 PB92-116722 Not available NTIS
National Inst. of Standards and Technology (NML),
Gaithersburg, MD. Temperature and Pressure Div.
Differences between Thermodynamic Temperature and t(IPTS-68) In the Range 230C to 660C.

Final rept. R. E. Edsinger, and J. F. Schooley. 1989, 12p Pub. in Metrologia 26, p95-106 1989.

Keywords: \*Temperature scales, Temperature measurement, Melting points, Aluminum, Uncertainty, Comparison, Reprints, International Practical Temperature Scale of 1968, Kelvin Thermodynamic Temperature Scale, Gas thermometry, IPTS-68.

Determination of the differences between the Kelvin Thermodynamic Temperature Scale (KTTS) and the International Practical Temperature Scale of 1968 (IPTS-68) in the range from 230 C to 660 C has been accomplished by gas thermometry. The estimated random uncertainty of the results ranges from + or - 0.005 C to + or - 0.008 C; the major uncertainties appear to lie in the determination of the volume of the gas bulb and the determination of its IPTS-68 temperature. The present results differ noticeably from earlier gas-thermometric determinations in the range of temperature overlap. The value found for the thermody-namic temperature of the freezing point of Al is (660.342 + or - 0.015) C.

PB92-116870 Not available NTIS Notional Inst. of Standards and Technology (NML), Boulder, CO. Time and Frequency Div.

Test of the Linearity of Quantum Mechanics by rf Spectroscopy of the (9)Be(+) Ground State. Final rept.

Final rept.
D. J. Heinzen, J. J. Bollinger, W. M. Itano, S. L. Gilbert, and D. J. Wineland. 1990, 3p
See also PB90-205899. Sponsored by Air Force Office of Scientific Research, Bolling AFB, DC., and Office of Naval Research, Arlington, VA.
Pub. in Proceedings of Rochester Conference on Coherence and Quantum Optics (6th), Rochester, NY., June 26-28, 1989, p479-481 1990.

Keywords: \*Quantum mechanics: \*Beryllium 9, Nuclear magnetic resonance, Radiofrequency spectrosco-py, Frequency standards, Ground state, Beryllium ions, Linearity, Tests, Reprints, Ion storage, Penning traps.

A frequency standard based on an rf hyperfine resonance in the ground state of (9)Be(1+) ions is used to set limits on possible nonlinearities in quantum me-

chanics. A limit of 2.4 x 10 to the -20 power eV is placed on the size of a possible nonlinear correction to the (9)Be(1+) nuclear Hamiltonian.

101,727 PB92-117118 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Ionizing Radiation Div. Novel Radiation Dosimetry Systems.

Final rept.

W. L. McLaughlin. 1991, 25p Pub. in Proceedings of International Symposium on High Dose Dosimetry for Radiation Processing, Vienna, Austria, November 5-9, 1990, p3-27 1991.

Keywords: \*Dosimeters, Electron spin resonance, Free radicals, Luminescence, Polymeric films, Optical activity, Alanines, Reprints, Dye dosimeters, Quartz dosimeters, Telemetering dosimetry, Telemetering dosimetry, Radiochromic dyes, Radiation processing.

New developments of high dose dosimetry systems have led to a number of improved adaptations of exist-ing dosimeters and several promising innovations. These systems include the following: thin film and polmeric 'radiochromic' systems; liquid and gel phase ra-diochromic systems; free radical systems analyzed by either electron spin resonance (ESR), color complex spectrophotometry, selective electrode potentiometry, or luminescence analysis; saccharide solutions analyzed by ESR or optical rotation measurement; blea-chable aqueous dye solutions or dye films analyzed by visible spectrophotometry; inorganic solid state sensors, such as SiO2, by potentiometric methods or ESR analysis; telemetering dosimetry systems based on laser beam analysis of radiochromic sensors.

01.728 PB92-117134 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Ionizing Radiation Div. Temperature Dependence of Radiochromic Film

Dosimeters.

Final rept.
W. L. McLaughlin, J. C. Humphreys, W. Z. Ba, H. M. Khan, M. Al-Sheikhly, and W. J. Chappas. 1991, 12p Pub. in Proceedings of International Symposium on High Dose Dosimetry for Radiation Processing, Vienna, Austria, November 5-9, 1990, p305-316 1991.

Keywords: \*Photographic film dosemeters, \*Film dosimetry, \*Dosimeters, Temperature dependence, Gamma radiation, Polymeric films, Reprints, Radiochromic dyes, Radiation processing.

Three types of transparent radiochromic films, two forming a blue image and one a red image, are now widely used in high dose dosimetry. These are FWT-60-00, a free standing nylon base film (nominal aborbed dose range: 1-50 kGy) which is usually measured at 605 and 510 nm wavelengths, GafChromic dosimetrs and sea and sea before the forming dose. simetry media, a coated polyester film (nominal dose range: 0.05-30 kGy), which is measured at a variety of visible wavelengths from 675 down to 400 nm, and Riso B3, a free standing polyvinylbutyral base film (nominal absorbed dose range 1-200 kGy) which is measured at a single wavelength, 554 nm. Each of these film types is also supplied in other forms for spe-cial applications and different useful dose ranges, so that the systems are now able to measure doses and make radiographic images (without development) over a wide dynamic range, namely 10 to 200,000 Gy, with reasonable precision, nominally + or - 3% at 95% confidence limits, without appreciable dose rate dependence. The high resolution radiographic images can be used for archival dose distribution records.

101,729 PB92-126572 PB92-126572 PC A03/MF A01 National Inst. of Standards and Technology (PL), Gaithersburg, MD. Interpretation of the SI for the United States and

Metric Conversion Policy for Federal Agencies.

Final rept. B. N. Taylor. Oct 91, 20p NIST/SP-814 Also available from Supt. of Docs. See also PB92-

Keywords: \*International system of units, \*Metric system, Units of measurement, Policies, Federal agen-

The National Institute of Standards and Technology (NIST) Special Publication replaces National Bureau of Standards (NBS) Letter Circular LC1132 published April 19, 1982. It reprints the Department of Commerce, NIST, Federal Register notice of December 20, 1990 titled 'Metric System of Measurement; Interpreta-tion of the International System of Units for the United States' (the International System of Units, abbreviated SI, is the modernized metric system); the Department of Commerce, Office of the Secretary. Federal Register notice of January 2, 1991 titled 'Metric Conversion Policy for Federal Agencies'; and Executive Order 12770 issued by the President of the United States on July 25, 1991 titled 'Metric Usage in Federal Govern-ment Programs.' The first Federal Register notice re-states the Department of Commerce's interpretation of the International System of Units for the United States that was last published by the Department in 1982; the second revises the Code of Federal Regulations (CFR) to remove the voluntary aspect of the conversion to the metric system of measurement for Federal agencies; and the Executive Order provides Presidential authority and direction for the use of the metric system of measurement by Federal departments and agencies in their programs. Also included is a diagram that shows graphically how the 19 SI derived units with special names are derived in a coherent manner from the SI base and supplementary units.

# PROBLEM-SOLVING INFORMATION FOR STATE & LOCAL GOVERNMENTS

#### Police, Fire, & Emergency Services

101,730 PB91-216796 PB91-216796 PC A04/MF A01 Herndom Group, Inc., Chapel Hill, NC. First Pass at Computing the Cost of Fire Safety in a Modern Society. W. P. Meade. Jun 91, 51p NIST/GCR-91/592 Contract NIST-525BNB1C6678 Sponsored by National Inst. of Standards and Technology (BFRL), Gaithersburg, MD.

Keywords: \*Fire safety, \*Cost estimates, US NIST, Residential buildings, Commercial buildings, Research management, Economic analysis, Insurance, Con-

The report provides an estimate of the total annual dollar costs of establishing and maintaining fire safety in 20th-Century United States. The cost of fire safety estimate is needed to serve as a basis for evaluating the benefits and appropriateness of current and pro-posed fire research programs of NIST. This was a rela-tively modest effort to obtain a first-order estimate of these costs and much of what is reported in these two reports is anecdotal. Nonetheless, the central conclusions one comes to in reading them are that the burden of fire on our society is substantially greater than previously realized and that significant reductions in this burden may be readily achievable through the continued development of fire science and the rapid transfer of fire research results. These findings are particularly relevant as the U.S. economy and its manufacturing infrastructure adjust to the competitive challenges of the global marketplace.

# SPACE TECHNOLOGY

#### **Astronautics**

101,731 PB91-144352 PC A04/MF A01 National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Robot Systems Div. Short-Term Evolution for the Flight Telerobotic Servicer.

R. Lumia. Dec 90, 61p NISTIR-4463

Keywords: \*Robotics, \*Teleoperators, \*Remote manipulator system, Space maintenance, Automatic control, Control systems design, Computer vision, Automation, Space station servicing, Space telerobotics, Flight telerobotic servicer.

The document identifies near term technology developments which would have significant impact on the evolution of the FTS toward autonomous operation. Analysis of anticipated FTS tasks is used to identify operations that might be performed autonomously rather than in a purely teleoperated fashion. Alternative techniques for automating these operations are then described. A discussion of FTS long term evolution is included as an appendix.

101,732

PB91-185090 PC A06/MF A01

National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Robot Systems Div.

Recommended Fine Positioning Test for the Development Test Flight (DTF-1) of the NASA Flight

Telerobotic Servicer (FTS).

N. Dagalakis, A. J. Wavering, and P. Spidaliere. Feb 91, 124p NISTIR-4478

Prepared in cooperation with National Aeronautics and Space Administration, Greenbelt, MD. Goddard Space Flight Center.

Keywords: \*Spacecraft maintenance, \*Telerobotics, \*Positioning, \*Flight tests, Robots, Robot sensors, Robot arms, Standards, Off line systems, Computer programming, DTF-1(Development Test Flight), NASA(National Aeronautics and Space Administration), FTS(Flight Telerobotic Servicer).

The purpose of the report is to propose test procedures for the NASA DTF (Development Test Flight)-1 positioning tests of the FTS (Flight Telerobotic Servicer). The unique problems associated with the DTF-1 mission are discussed, standard robot performance tests and terminology are reviewed and a very detailed description of flight-like testing and analysis is presented. The major technical problem associated with DTF-1 is that only one position sensor can be used, which will be fixed at one location, with a working volume which is probably smaller than some of the robot errors to be measured. Radiation heating of the arm and the sensor could also cause distortions that would interfere with the test. Two robot performance testing committees have established standard testing procedures relevant to the DTF-1. Due to the technical problems associated with DTF-1 these procedures cannot be applied directly. These standard tests call for the use of several test positions at specific locations. Only one position, that of the position sensor, can be used by DTF-1. Off-line programming accuracy might be impossible to measure and in that case it will have to be replaced by forward kinematics accuracy.

## **Extraterrestial Exploration**

101.733

PB91-237875 Not available NTIS National Inst. of Standards and Technology (NML), Gaithersburg, MD. Ionizing Radiation Div. Possible Use of Pattern Recognition for the Analy-

sis of Mars-Rover X-ray-Fluorescence Spectra. Final rept.

L. I. Yin, J. I. Trombka, S. M. Seltzer, R. G. Johnson, and J. A. Philpotts. 1989, 8p Pub. in Jnl. of Geophysical Research 94, nNB10 p3611-3618 1989.

Keywords: \*Mars sample return missions, \*Mars surface samples, \*X-ray fluorescense analysis, \*Pattern recognition, \*Soils, Chemical analysis, Reprints.

In the Mars Sample Return Mission, a rover vehicle may be used to collect and select samples from differ-ent locations on the Martian surface to be brought back to earth for laboratory studies. It is anticipated that an in-situ energy-dispersive x-ray fluorescence (XRF) spectrometer will be on-board the rover. In such a mission, sample selection is of higher priority than insitu quantitative chemical analysis. With this in mind, a simple, direct and speedy pattern-recognition method

## SPACE TECHNOLOGY

#### **Extraterrestial Exploration**

has been developed as an alternative to detailed chemical analysis of the XRF spectra. The authors present and discuss laboratory demonstrations of the efficacy of this pattern-recognition technique in the analysis of many XRF spectra obtained from a series of geological samples, including a simulated Martian

#### Manned Spacecraft

101,734 PB91-184804 PC A05/MF A01 National Inst. of Standards and Technology (NML), Boulder, CO. Chemical Engineering Science Div. Heat Transfer in a Compact Heat Exchanger Containing Rectangular Channels and Using Helium Gas.

Olson, Jan 91, 99p NISTIR-3959
See also PB91-107573. Sponsored by National Aeronautics and Space Administration, Hampton, VA. Langley Research Center.

Keywords: \*Heat exchangers, \*Heat transfer, Friction factor, Channel flow, Heat transfer coefficient, Reynolds number, Turbulent flow, Experimental data, Heat Temperature distribution. Nusselt number. Helium, Mass flow, National Aerospace Plane.

Development of a National Aerospace Plane (NASP) which will fly at hypersonic speeds, requires novel cooling techniques to manage the anticipated high heat fluxes on various components. The author has constructed a compact heat exchanger consisting of 12 parallel, rectangular channels in a flat piece of com-mercially pure nickel. The channel specimen was ra-diatively heated on the top side at heat fluxes of up to W/sq cm insulated on the back side, and cooled with helium gas flowing in the channels at 3.5 to 7.0 MPa and Reynolds numbers of 1400 to 28,000. The measured friction factor was lower than that of the accepted correlation for fully developed turbulent flow, although our uncertainty was high due to uncertainty in the channel height and a high ratio of dynamic pressure to pressure drop. The measured Nusselt number, when modified to account for differences in fluid properties between the wall and the cooling fluid, agreed with past correlations for fully developed turbulent flow in channels. Flow nonuniformity from channel-to-channel was as high as 12% above and 19% below the mean flow.

101,735 PB91-216606 PC A05/MF A01 National Inst. of Standards and Technology (BFRL), Gaithersburg, MD. Material Flammability Test Assessment for Space

Station Freedom.
T. J. Ohlemiller, and K. M. Villa. Jun 91, 79p NISTIR-4591, NASA-CR-187115
Sponsored by National Aeronautics and Space Administration, Cleveland, OH. Lewis Research Center.

Keywords: \*Spacecraft construction materials, \*Space stations, \*Flammability testing, Reduced gravity, Test methods, Fire tests, Ignition, Comparison, Space hazards, NASA, Graphs(Charts), US NIST.

The NASA Upward Flame Propagation test, which measures response to a well-defined laminar flame at the bottom of a test sample, is currently used to screen for flammability all materials intended for use in the interior of manned spacecraft. The response of a series of materials was compared in the test and in the standard NIST flammability tests (Cone Calorimeter for rate of heat release and LIFT tests for ignitability and lateral flame spread). The goal was to see if these differing flammability assessment approaches provide comparable information on the potential hazards of a material. At the present, a firm relation between the behavior in the NASA test and in the NIST tests has not been established. Recommendations are given for future testing.

Spacecraft Trajectories & Flight Mechanics

101,736 PB91-175166

Not available NTIS

National Inst. of Standards and Technology (NML), Boulder, CO. Quantum Physics Div.

Orbit Determination and Gravitational Field Accuracy for a Mercury Transponder Satellite.

Final rept. M. A. Vincent, and P. L. Bender. 1990, 5p

Grant NAGW-822

Sponsored by National Aeronautics and Space Administration, Washington, DC.

Pub. in Jril. of Geophysical Research 95, nB13 p21,357-21,361, 10 Dec 90.

Keywords: \*Gravitational fields, \*Orbit calculation, \*Mercury(Planet), Mercury spacecraft, Range finding, Circular orbits, Polar orbits, Transponders, Librations,

Covariance studies were performed to investigate the orbit determination problem for a small transponder satellite in a nearly circular polar orbit with 4-hour period around Mercury. With X band and Ka band Doppler and range measurements, the analysis indicates that the gravitational field through degree and order 10 can be solved for from as few as 40 separate 8-hour arcs of tracking data. In addition, the Earth-Mer-cury distance can be determined during each ranging period with about 6-cm accuracy. The expected geoid accuracy is 10 cm up through degree 5, and 1 m through degree 8. The main error sources were the geocentric range measurement error, the uncertainties in higher degree gravity field terms, which were not solved for, and the solar radiation pressure uncertain-

Apparatus for Measurement of Thermal Conductivity of Insulation Systems Subjected to Extreme Temperature Differences. Final rept. W. P. Dube, L. L. Sparks, A. J. Slifka, and R. M. Bitsy. 1990, 7p

Sponsored by National Aeronautics and Space Administration, Hampton, VA. Langley Research Center. Pub. in Advances in Cryogenic Engineering (Materials), v36 p853-859 1990.

Keywords: \*Thermal insulation, \*Thermal conductivity, \*Test facilities, \*Spacecraft design, \*Thermal measurements, Thermal analysis, Thermal protection, Cryogenics, Temperature measurement, Heat transmission by the professional sections of the conductivity of the co sion, Heat transfer, Reprints.

Advanced aerospace designs require thermal insulation systems which are consistent with cryogenic fluids, high thermal loads, and design restrictions such as weight and volume. To evaluate the thermal performance of these insulating systems, an apparatus capable of measuring thermal conductivity using extreme temperature differences (27 to 1100 K) is being developed. The system is described along with estimates of precision and accuracy in selected operating conditions. Preliminary data are presented. conditions. Preliminary data are presented.

## TRANSPORTATION

## **Unmanned Spacecraft**

101,737

PB91-161950 Not available NTIS National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Scientific Computing Div.

Probe Waveforms and the Reconstruction of Structural Dynamic Green's Functions.

Final rept. A. S. Carasso. 1991, 5p

Contracts AFOSR-ISSA-88-0036, ONR-N00014-89-F-0013

Sponsored by Air Force Office of Scientific Research, Bolling AFB, DC., and Office of Naval Research, Arlington, VA.

Pub. in AIAA Jnl. 29, n1 p114-118 Jan 91.

Keywords: \*Large space structures, Dynamic structural analysis, Greens function, Waveforms, Pulses, Reprints, Deconvolution.

Experimental identification of dynamic behavior in linear structural systems can be achieved by exciting the structure with a specifically synthesized pulse, and reconstructing the relevant dynamic Green's function by deconvolution of the measured response. The reconstruction procedure involves the solution of an illposed integral equation in the presence of noise. The paper underlines the rich variety of infinitely divisible pulse shapes that may be used while still retaining a pulse shapes that may be used while still retaining shape is necessary to allow for possible perturbations caused by interfacing devices that convert electrical voltages into mechanical forces. A numerical experiment, using synthetic noisy data, shows that the reconstruction procedure remains effective even when the probe waveform deviates strongly from the preferred unimodal shape. A dispersive structural network that may be representative of a large space structure is used as an illustrative example.

#### General

101,738

PB91-162016 Not available NTIS National Inst. of Standards and Technology (NML), Boulder, CO. Chemical Engineering Science Div.

## Air Transportation

101,739

PB92-112226 PC A05/MF A01 National Inst. of Standards and Technology (MSEL),

Gaithersburg, MD. Metallurgy Div.
Static and Dynamic Strength Tests on Electrical Conductor Cables Specified for Airport Landing Structures. Final rept.

R. J. Fields, S. R. Low, and D. E. Harne. 27 Oct 88, 82p NISTIR-88-3884

Sponsored by Federal Aviation Administration, Washington, DC. Navigation and Landing Div.

Keywords: \*Static tests, \*Strength, \*Electric wire, \*Landing aids, Electric conductors, Dynamic tests, Experimental data, Test facilities, Displacement, Strains, Mechanical properties, Fatigue(Mechanical), Wire, Impact tests, Loads(Forces), Mechanical tests.

The report covers a series of static and dynamic tests on electrical conductors specified for use in landing aids on airport runways carried out by NIST for the Federal Aviation Administration. The structures are intended to be frangible so that they will break up readily if impacted, thus minimizing damage to the impacting aircraft. While the structures are frangible, they contain electrical cables which, due to the requirement of electrical conduction, are not frangible. In an actual impact, these cables do not break readily and tend to wrap around the aircraft. The tests authorized by the FAA were carried out to assess the force required to break through various types of FAA specified cables by a simulated aircraft impact. Furthermore, the effectiveness of using break-away connectors was evaluated to determine if they would reduce the total load on an impacting aircraft. In order to correctly design the dynamic test apparatus, it was necessary to know the approximate, expected load levels and cable elongations at fracture. Therefore a series of quasi-static tests were performed on the cables and break-away connectors. The report describes these quasi-static tests as well as the construction and application of the dynamic test apparatus.

101.740

Management.

PC A06/MF A02 PB92-112580 National Inst. of Standards and Technology (NCSL), Gaithersburg, MD.

Galtnersburg, MD.

Prototyping the IRDS: An Airport Application.

A. P. Sani. Oct 91, 119p NISTIR-4688

See also PB89-136329. Sponsored by Univ. of Toronto, Mississauga (Ontario). Inst. for Land Information

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# TRANSPORTATION

## Air Transportation

Keywords: \*Geographic information systems, \*Data management, \*Airports, Software tools, Data bases, \*Information Resource Dictionary System, \*IRDS system, GIRDS system, Federal information processing standards.

The management of geographic information resources (GIRS) continues to be plagued by problems of monitoring, locating and controlling the array of geographic information in complex organizations. Software tools to support these functions are fundamental to any effort to maintain the integrity of geographic information as it changes. In addition, such tools are desirable when formalizing, then managing the integration of geographic information resources within an organization. One of the major approaches to the problem in the One of the major approaches to the problem in the area of database systems has been the development of the information resource dictionary (IRD) which contains meta-data. An Information Resource Dictionary System (IRDS) is a database of meta-data along with software and procedures for the creation and mainte-nance of the IRD. In 1989 the American National Standards Institute (ANSI) X3.138-1988 IRDS (ANSI-IRDS) was adopted as Federal Information Processing Standard 156 by the United States Government. ANSI-IRDS is intended to support the definition, manage-ment and control of mete-data. The study presents the first known attempt to actually apply ANSI-IRDS in the geographic information management domain.

#### **Railroad Transportation**

PB91-222653 PC A03/MF A01
National Inst. of Standards and Technology (MSEL),
Boulder, CO. Materials Reliability Div.
Residual Stress Detection in Railroad Wheels: An
Ultrasonic System Using EMATs (ElectromagneticAcoustic Transducers), Report No. 23.
Final rept. Sep 85-Dec 90.
R. E. Schramm, A. V. Clark, D. V. Mitrakovic, S. R.
Schaps, and T. J. McGuire. May 91, 47p NISTIR3968 101,741 PB91-222653

3968

Contract DTFR-53-89-X-00018
See also PB91-222661. Sponsored by Federal Railroad Administration, Washington, DC. Office of Research and Development.

Keywords: \*Ultrasonic tests, \*Railroad cars, \*Wheels, \*Residual stress, Detection, Inspection, Accident prevention, Nondestructive tests, Signal processing, Transducers, Surface waves,

The report covers research performed by the National Institute of Standards and Technology for the Federal Railroad Administration. The report covers a project by the Materials Reliability Division (formerly the Fracture and Deformation Division) to develop and build a system to detect and measure residual stress in the rims of railroad wheels. Acoustic birefringence is the underlying principle of operation. This is a measure of the relative difference in the propagation times of two shear waves polarized in radial and circumferential di-rections. Measurements employ an EMAT (electromagnetic-acoustic transducer) as an ultrasonic probe. magnetic-acoustic transducer) as an ultrasonic probe. This type of transducer requires little or no surface preparation and no acoustic couplant. The system operates in a pulse-echo mode. A short burst of shear horizontal waves travels through the rim thickness. The rotation of the EMAT determines the orientation of the polarization vector, radial or circumferential. Precise timing of echoes in both directions reveals the degree of birefringence. Changes are due to both stress state and metalluroical texture. Initial tests indistress state and metallurgical texture. Initial tests indicate it may be possible to separate these two.

101,742 PB91-222661 PC A04/MF A01 National Inst. of Standards and Technology (MSEL), Boulder, CO. Materials Reliability Div. Tread Crack Detection in Railroad Wheels: An UI-

trasonic System Using EMATs (Electromagnetic-Acoustic Transducers). Report No. 22.
Final rept. Sep 85-Dec 90.
R. E. Schramm, A. V. Clark, D. V. Mitrakovic, Y.
Cohen, P. J. Schull, and S. R. Schaps. May 91, 69p
NISTIR-3967 Contract DTFR-53-89-X-00018

See also PB91-222653. Sponsored by Department of Transportation, Federal Railroad Administration, Washington, DC. Office of Research and Develop-

Keywords: \*Ultrasonic tests, \*Railroad cars, \*Wheels, \*Cracks, Fractures(Materials), Detection, Treads, Nondestructive tests, Accident prevention, Inspection, Signal processing.

The report covers research performed by the National Institute of Standards and Technology (NIST) for the Federal Railroad Administration (FRA). The report covers a project by the Materials Reliability Division (formerly the Fracture and Deformation Division) to develop and build an ultrasonic system to detect cracktype flaws in the tread of railroad wheels. To achieve fully automatic operation, the sensor is built into the rail so testing occurs as the train rolls past. Signal analysis takes place in real time. The ultrasonic probe is an EMAT (electromagnetic-acoustic transducer). As con-

figured here, the EMAT has a small footprint, and, due to its principle of operation, it does not require any acoustic couplant. The system operates in a pitchcatch mode. A short burst of Rayleigh (surface) waves travels around the wheel tread, and an echo indicates a flaw's presence and size. Testing was performed on both a short track in the NIST laboratory and the full-scale facilities of the Transportation Test Center (TTC) in Pueblo, Colorado. The report documents the design, construction, and testing of the system. It is also to serve as an operational guide for the equipment being delivered to the FRA.

### **Road Transportation**

101.743

PB91-157156 PC A03/MF A01 National Inst. of Standards and Technology (NEL), Gaithersburg, MD. Robot Systems Div. New Approach to Vision and Control for Road Fol-

lowing. D. Raviv, and M. Herman. Jan 91, 46p NISTIR-4476 Prepared in cooperation with Florida Atlantic Univ., Boca Raton.

Keywords: \*Robot dynamics, \*Control systems, \*Computer vision, \*Ground vehicles, Robots, Optical processing, Automous navigation, Image processing.

The paper deals with a new quantitative, vision-based approach to road following. It is based on the theoretical framework of the recently developed optical flow-based visual field theory. By building on this theory, the authors suggest that motion commands can be generated discrete force the constitution of the constitution ated directly from a visual feature, or cue, consisting of the projection into the image of the tangent point to the reprojection into the image of the tangent point to the edge of the road, along with the optical flow of this point. Using this cue, they suggest several different vision-based control approaches. There are several advantages to using this visual cue: it is extracted directly from the image, i.e., there is no need to reconstitution. struct the scene; for many road following situations this is the only necessary visual cue; only the horizontal component of the optical flow of the tangent point needs to be extracted; it has a scientific basis, i.e., the described techniques are not ad-hoc; and the related computations are relatively simple and thus suitable for real-time applications. For each control approach, they derive the value of the related steering com-



# SAMPLE ENTRY

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Proposed Standard Practice for Assessing the Performance of Gas-Phase Air Cleaning Equipment 100,905 PB91-167353

Author name(s) Title

NTiS order number

Abstract number

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PQq1-147918
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# SAMPLE ENTRY

#### Air Pollution & Control

2-METHYLPROPANE

AC LOSSES

**ACCESS** 

Proposed Standard Practice for Assessing the Performance of Gas-Phase Air Cleaning Equipment PB91-167353 100,905 Keyword term Title

NTIS order number

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ACOUSTIC VELOCITY

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Title

NTIS order number

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AD-A240 610/6 70 PC A03/MF A01

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AD-A240 613/0 100,622 PC A05/MF A01

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400.620 PC A05/MF A01

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AD-A230 438/4

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AD-A230 957/3

Vibrational Spectra of Molecular lons Isolated in Solid Neon. IV.NO(+), NO(-), ONNO(+), aNd ONNO(-). AD-A230 957/3 PC A03/MF A01

AD-A231 778/2

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AD-A231 778/2

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AD-A233 961/2

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AD-A234 043/8

Production and Spectroscopy of Small Polyatomic Molecular Ions Isolated in Solid Neon. AD-A234 043/8 100,245 PC A03/MF A01

AD-A234 083/4

Ada Compiler Validation Summary Report: DDC International A/S, DACS VAX/VMS to 80186 Bare Ada Cross Compiler System, Version 4.6, VAX 8530 (Host) to Bare Board ISBC 186/93A (Host), 90112951.11079.

AD-A234 083/4 PC A05/MF A01 100,608 PC A05/MF A01

AD-A234 118/8

Ada Compiler Validation Summary Report: Certificate Number: 901129S1.11112 DDC International A/S DACS

80386 DMS/OS Ada Compiler System, Version 4.6 IBM PS/2 Model 80-311 = > IBM PS/2 Model 80-311. AD-A234 118/8 100,609 PC A06/MF A01

AD-A234 323/4

Ada Compiler Validation Summary Report: Certificate Number: 901129S1.11050 DDC International A/S DACS VAX/VMS Native Ada Compiler System, Version 4.6 VAX VAX 8530. AD-A234 323/4

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100.610 PC A04/MF A01

Ada Compiler Validation Summary Report: Digital Equipment Corporation, VAX Ada, Version 2.2, BAX 8800 (Host) t VAX MicroVAX II Running VAXELN Version 4.1 (Target), 901109S1.11054.

AD-A234 350/7 100.611 PC A04/MF A01

AD-A234 380/4

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100,612 PC A03/MF A01

AD-A234 438/0

Ada Compiler Validation Summary Report: Certificate Number: 901129S1.11077 DDC International A/S DACS VAX/VMS to 80186 Bare Ada Cross Compiler System with Rate Monotonic Scheduling, Version 4.6 VAX 8530 = > Bare Board iSBC/03A.

AD-A234 438/0 100,613 PC A06/MF A01

AD-A234 439/8

Ada Compiler Validation Summary Report: Certificate Number: 901129S1.11075 DDC International A/S DACS 80386 UNIX V Ada Compiler System, Version 4.6 ICL DRS300 = > ICL DRS300.

AD-A234 439/8 100,614 PC A04/MF A01

AD-A234 529/6

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AD-A239 715/6

Ada Compiler Validation Summary Report. Certificate Number: 91051051.11161 UNISYS Corporation, UCS Ada, Version 1R1, 2200/600 (Host and Target). Revision. AD-A239 715/6 100,616 PC A06/MF A02

AD-A239 729/7

Vibrational Spectra of Molecular Ions Isolated in Solid Neon. 7. CO(+ ), C2O2(+ ), and C2O2(-). AD-A239 729/7 100,250 Not available NTIS

Ada Compiler Validation Summary Report: Certificate Number: 910626S1.11179 U.S. Navy Ada/M, Version 4.0 (OPTIMIZE) VAX 11/785 = AN/AYK-14 (Bare Board) AD-A240 511/6 700,617 PC A05/MF A01

AD-A240 512/4

Ada Compiler Validation Summary Report: Certificate Number 91070551.11192 InterAct Corporation InterAct Ada Mips Cross-Compiler System, Release 2.0 MicroVAX 3100 Cluster = Lockheed Sanders STAR MVP R3000/ Cluster = > Lockheed Sa R3010 board (Bare Machine).

100.618 PC A04/MF A01 AD-A240 512/4

AD-A240 610/6

Ada Compiler Validation Summary Report: Certificate Number: 91050281.11158 DDC International A/S, DACS VAX/VMS to 80860 Bare Ada Cross Compiler System, Version 4.6.1, VAX 8530 (Host) to Tadpole Technology PLC TP860M (Bare Board) (Target).

AD-A240 610/6 70 PC A03/MF A01

AD-A240 611/4

Ada Compiler Validation Summary Report: Certificate Number: 910626S1.11176 U.S. Navy, Ada/L, Version 4.0 (/

Optimize), VAX 11/785 (Host) to AN/UYJ-43 (Single CPU) (Bare Board) (Target).
AD-A240 611/4 100,620 PC A05/MF A01

AD-A240 612/2

Ada Compiler Validation Summary Report: Certificate Number: 910626S1.11174 U.S. Navy, Ada/M, Version 4.0 (/Optimize), VAX 8550, Running VAX/VMS Version 5.3 (Host) to AN/UYK-44 (EMR) (Bare Board) (Target), AD-A240 612/2 PC A05/MF A01

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(Target). AD-A240 613/0

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100,622 PC A05/MF A01

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AD-A240 763/3

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AD-A240 763/3

100,624 PC A05/MF A01

AD-A240 783/1

Ada Compiler Validation Summary Report: Certificate Number 91062651.11173 U.S. Navy Ada/L, Version 4.0 (/ Optimize) VAX 855 = AN/UYK-43 (EMR) (Bare Board). AD-A240 783/1 100,625 PC A05/MF A01

AD-A240 784/9

Ada Compiler Validation Summary Report: Certificate Number Number 910626S1.11172 U.S. Navy Ada/L, Version 4.0 (/Optimize) VAX 8550 = AN/UYK-43 (Single CPU) (Bare Board).

AD-A240 784/9 100,626 PC A05/MF A01

AD-A240 785/6

Ada Compiler Validation Summary Report: Certificate Number: 91050251.11159 DDC International A/S DACS Sun-3/Sun0S to 68030 Bare Ada Cross Compiler System, Version 4.6.4, MRI IEEE 695 (BASIC-MODE) Sun-3/50 = Motorola MVME143 Board (68030/68882).

AD-A240 785/6 100,627 PC A03/MF A01

AD-A240 849/0

Ada Compiler Validation Summary Report. Certificate Number: 910502S1.11160 DDC International A/S DACS Sun-3/SunOS to 68030 Bare Ada Cross Compiler System, Version 4.64, MRI IEEE 695 (SECURE MODE) Sun-3/50 = > Motorola MVME143 Board (68030/68882). AD-A240 849/0 100,628 PC A03/MF A01

AD-A240 850/8

Ada Compiler Validation Summary Report. Certificate Number: 910626S1.11177 U.S. NAVY Ada/L, Version 4.0 (/OPTIMIZE) VAX 11/785 = > AN/UYK-43 (EMR) (Bare Board). AD-A240 850/8 100,629 PC A05/MF A01

AD-A242 029/7

Liquid and Solid Ion Plasmas. AD-A242 029/7 101.592 PC A02/MF A01

AD-A242 030/5

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Ada Compiler Validation Summary Report: Certificate Number: 91051751.11163 U.S. Navy, AdaVAX, Version 5.0, (/NO OPTIMIZE) VAX 8350 (Host and Target). AD-A242 268/1 100,630 PC A08/MF A02

AD-A242 269/9

Ada Compiler Validation Summary Report: Certificate Number: 91051751.11162 U.S. Navy, AdaVAX, Version 5.0, (/OPTIMIZE) VAX 8600 (Host and Target). AD-A242 269/9 100,631 PC A05/MF A01 AD-A242 270/7

Ada Compiler Validation Summary Report: Certificate Number: 91051751.11165 U.S. Navy, AdaVAX, Version 5.0 (/NO-OPTIMIZE), VAX 11/785 (Host and Target). AD-A242 270/7 100,632 PC A04/MF A01

AD-A242 273/1

Ada Compiler Validation Summary Report: Certificate Number: 91051751.11164 U.S. Navy, AdaVAX, Version 5.0, (/OPTIMIZE), VAX11/785 (Host and Target). AD-A242 273/1 100,633 PC A04/MF A01

AD-A242 609/6

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AD-A242 609/6 100,634 PC A05/MF A01

AD-A242 816/7

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AD-A242 896/9

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AD-A242 956/1

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AD-A242 956/1 101,204 PC A07/MF A02

AD-A243 049/4

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AD-A243 093/2

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## **ALABAMA**

#### Auburn

Auburn University Ralph Brown Draughon Library (1873)

# **Birmingham**

Birmingham Public Library (1895)
Birmingham-Southern College Library (1932)
Jefferson State Community College James B. Allen Library (1970)
Samford University Library Harwell G. Davis Library (1884)

# Enterprise

Enterprise State Junior College Learning Resources Center (1967)

# **Fayette**

Brewer State Junior College Learning Resources Center Library (1979)

### **Florence**

University of North Alabama Collier Library (1932)

# Gadsden

Gadsden Public Library (1963)

### Huntsville

University of Alabama in Huntsville Library (1964)

# **Jacksonville**

Jacksonville State University Houston Cole Library (1929)

## Mobile

Mobile Public Library (1963) Spring Hill College Thomas Byrne Memorial Library (1937) University of South Alabama Library (1968)

### Montgomery

Alabama Public Library Service (1984) Alabama Supreme Court and State Law Library (1884) Aubum University at Montgomery Library (1971) REGIONAL Air University Library Maxwell Air Force Base (1963)

## Normal

Alabama Agricultural and Mechanical University J. F. Drake Memorial Learning Resources Center (1963)

## Troy

Troy State University Library (1963)

### Tuscaloosa

University of Alabama Amelia Gayle Gorgas Library (1860) REGIONAL University of Alabama School of Law Library (1967)

## Tuskegee

Tuskegee University Hollis Burke Frissell Library (1907)

#### **ALASKA**

# **Anchorage**

Anchorage Law Library (1973)
Anchorage Municipal Libraries Z. J. Loussac Public Library (1978)
University of Alaska at Anchorage Library (1961)
U.S. Alaska Resources Library (1981)
U.S. District Court Law Library (1983)

### **Fairbanks**

University of Alaska Elmer E. Rasmuson Library (1922)

#### Jungau

Alaska State Library (1900) University of Alaska-Juneau Library (1981)

#### Ketchikan

Ketchikan College Library (1970)

### AMERICAN SAMOA

# Pago Pago

American Samoa Community College Learning Resources Center (1985)

# **ARIZONA**

## Coolldge

Central Arizona College Instructional Materials Center (1973)

## Flagstaff

Northern Arizona University Cline Library (1937)

### Glendale

Glendale Public Library (1986)

#### Holbrook

Northland Pioneer College Learning Resources Center (1985)

#### Mesa

Mesa Public Library (1983)

### **Phoenix**

Department of Library Archives, and Public Records (unknown) REGIONAL Grand Canyon University Fleming Library (1978) Phoenix Public Library (1917) U.S. Court of Appeals 9th Circuit Library (1984)

#### Prescott

Yavapai College Library (1976)

#### Tempe

Arizona State University College of Law Library (1977) Arizona State University Hayden Library (1944)

#### Tucson

Tucson Public Library (1970) University of Arizona Library (1907) REGIONAL

#### Yuma

Yuma County Library (1963)

# **ARKANSAS**

## Arkadelphla

Ouachita Baptist University Riley Hickingbotham Library (1963)

### Batesville

Arkansas College Library (1963)

#### Clarksville

University of the Ozarks Dobson Memorial Library (1925)

## Conway

Hendrix College Olin C. Bailey Library (1903)

# **Fayetteville**

University of Arkansas Mullins Library (1907) University of Arkansas School of Law Library Robert A. Leflar (1978)

### Little Rock

Arkansas State Library (1978) REGIONAL
Arkansas Supreme Court Library (1962)
Central Arkansas Library System Main Library (1953)
University of Arkansas at Little Rock Library Ottenheimer Library (1973)
University of Arkansas at Little Rock Pulaski County Law Library
(1979)

## Magnolla

Southern Arkansas University Magale Library (1956)

# Monticello

University of Arkansas at Monticello Library (1956)

### Pine Bluff

University of Arkansas at Pine Bluff Watson Memorial Library (1976)

## Russellville

Arkansas Technical University Tomlinson Library (1925)

## Searcy

Harding University Brackett Library (1963)

## State University

Arkansas State University Dean B. Ellis Library (1913)

# Walnut Ridge

Southern Baptist College Felix Goodson Library (1967)

## CALIFORNIA

## **Anahelm**

Anaheim Public Library (1963)

## Arcadla

Arcadia Public Library (1975)

#### Arcata

Humboldt State University Library (1963)

### Bakersfield

California State University Bakersfield Library (1974) Kern County, Beale Memorial Library (1943)

## Berkeley

University of California General Library (1907) University of California Boalt Law Library (1963)

#### Carson

California State University Dominguez Hills Library (1973) Carson Regional Library (1973)

#### Chico

California State University, Chico Merriam Library (1962)

#### Claremont

Government Publications and Microforms Department Honnold Library, Claremont College (1913)

## Compton

Compton Public Library (1972)

## **Culver City**

Culver City Public Library (1966)

#### Davis

University of California Shields Library (1953) University of California at Davis Law Library (1972)

### Downey

Downey City Library (1963)

#### Fresno

California State University, Fresno, Henry Madden Library (1962) Government Documents Department Library (1920)

#### **Fullerton**

California State University at Fullerton Library (1963)

### **Garden Grove**

Orange County Public Library (1963)

#### Gardena

County of Los Angeles Public Library (1966)

### Havward

California State University, Hayward Library (1963)

### **Huntington Park**

Huntington Park Library (1970)

## Inglewood

Inglewood Public Library (1963)

### Irvine

University of California at Irvine Main Library (1963)

#### La Jolla

University of California at San Diego Central University Library (1963)

#### Lakewood

Angelo Iacoboni Public Library (1970)

### Lancaster

Lancaster Library (1967)

## La Verne

University of La Verne College of Law Library (1979)

# Long Beach

California State University at Long Beach Library (1962) Long Beach Public Library (1933)

## Los Angeles

California State University, Los Angeles University Library (1956)
Los Angeles County Law Library (1963)
Los Angeles Public Library (1891)
Loyola Marymount University Charles Von der Ahe Library (1933)
Loyola Law School William M. Rains Law Library (1979)
Occidental College Library (1941)
Southwestern University School of Law Library (1975)
University of California, University Research Library (1932)
University of California, Los Angeles Law Library (1958)
University of Southern California Doheny Memorial Library (1933)
University of Southern California Law Library (1978)
U.S. Court of Appeals Ninth Circuit Library (1981)
Whittier College School of Law Library (1978)

#### Mallbu

Pepperdine University Payson Library (1963)

### Menlo Park

U.S. Geological Survey Library (1962)

## Montebello

Montebello Regional Library (1966)

### Monterey

U.S. Naval Postgraduate School Dudley Knox Library (1963)

## **Monterey Park**

Bruggemeyer Memorial Library (1964)

## Northridge

California State University at Northridge Oviatt Library (1958)

#### Norwalk

Norwalk Regional Library (1973)

### **Oakland**

Mills College Library (1966) Oakland Public Library (1923)

### Ontario

Ontario City Library (1974)

# Palm Springs

Palm Springs Public Library (1980)

### **Pasadena**

California Institute of Technology Millikan Memorial Library (1933) Pasadena Public Library (1963)

#### Pleasant HIII

Contra Costa County Library (1964)

## Redding

Shasta County Library (1956)

#### Rediands

University of Redlands Armacost Library (1933)

# **Redwood City**

Redwood City Public Library (1966)

#### Reseda

West Valley Regional Branch Library (1966)

### Richmond

Richmond Public Library (1943)

## Riverside

Riverside City and County Public Library (1947) University of California at Riverside Library (1963)

## Sacramento

California State Library (1895) REGIONAL
California State University Sacramento Library (1963)
Sacramento County Law Library (1963)
Sacramento Public Library (1880)
University of the Pacific McGeorge School of Law Library (1978)

### San Bernardino

Don A. Turner County Law Library (1984) San Bernardino County Library (1964)

# San Dlego

National University Law Library (1989)
San Diego County Law Library (1973)
San Diego County Library (1973)
San Diego Public Library (1895)
San Diego State University Library (1962)
University of San Diego Legal Research Center (1967)

### San Francisco

Golden Gate University School of Law Library (1979)

University of California Hastings College of Law Library (1972) San Francisco Public Library (1889)
San Francisco State University J. Paul Leonard Library (1955) Supreme Court of California Library (1979)
U.S. Court of Appeals Ninth Circuit Library (1971)
University of San Francisco Richard A. Gleeson Library (1963)

#### San Jose

San Jose State University Clark Library (1962)

### San Leandro

San Leandro Community Library Center (1961)

## San Luis Obispo

California Polytechnic State University Robert E. Kennedy Library (1969)

### San Mateo

College of San Mateo Library (1987)

## San Rafael

Marin County Free Library (1975)

## Santa Ana

Orange County Law Library (1975) Santa Ana Public Library (1959)

### Santa Barbara

University of California at Santa Barbara Library (1960)

### Santa Clara

Santa Clara University Orradre Library (1963)

# Santa Cruz

University of California at Santa Cruz McHenry Library (1963)

### Santa Rosa

Sonoma County Library (1896)

### Stanford

Stanford University Libraries (1895) Stanford University Robert Crown Law Library (1978)

## Stockton

Public Library of Stockton and San Joaquin County (1884)

### **Thousand Oaks**

California Lutheran University Pearson Library (1964)

## **Torrance**

Torrance Public Library (1969)

### Turlock

California State University, Stanislaus Library (1964)

## Vallejo

Solano County Library John F. Kennedy Library (1982)

### Valencia

Valencia Regional Library (1972)

#### Ventura

Ventura County Library Services Agency (1975)

#### Visalia

Tulare County Free Library (1967)

### Walnut

Mount San Antonio College Library (1966)

## West Covina

West Covina Regional Library (1966)

#### Whittler

Whittier College Wardman Library (1963)

### **COLORADO**

### Alamosa

Adams State College Library (1963)

### Aurora

Aurora Public Library (1984)

### Boulder

University of Colorado at Boulder Norlin Library (1879) REGIONAL University of Colorado School of Law Library (1988)

## Colorado Springs

Colorado College Tutt Library (1880) University of Colorado at Colorado Springs Library (1974) U.S. Air Force Academy Library (1956)

### Denver

Auraria Library (1978)
Colorado Supreme Court Library (1978)
Denver Public Library (1884) REGIONAL
Department of the Interior Library (1962)
Regis College Dayton Memorial Library (1915)
U.S. Courts Library (1973)

University of Denver Penrose Library (1909)
University of Denver College of Law Westminster Law Library (1978)

### Fort Collins

Colorado State University Libraries (1907)

### Golden

Colorado School of Mines Arthur Lakes Library (1939)

### **Grand Junction**

Mesa State College Tomlinson Library (1978) Mesa County Public Library (1975)

## Greelev

University of Northern Colorado James A. Michener Library (1966)

### Gunnison

Western State College Leslie J. Savage Library (1932)

#### La Junta

Otero Junior College Wheeler Library (1963)

#### Lakewood

Jefferson County Public Library Lakewood Library (1968)

### Pueblo

Pueblo Library District (1893) University of Southern Colorado Library (1965)

## CONNECTICUT

## **Bridgeport**

Bridgeport Public Library (1884)
University of Bridgeport School of Law Library Wahlstrom Library (1979)

## Danbury

Western Connecticut State University Ruth A. Haas Library (1967)

## Danlelson

Quinebaug Valley Community College Audrey P. Beck Library (1968)

# Enfleld

Enfield Central Library (1967)

#### Hartford

Connecticut State Library (unknown) REGIONAL Hartford Public Library (1945)

Trinity College Library (1895) University of Connecticut School of Law Library (1978)

## Middletown

Wesleyan University Olin Library (1906)

## Mystlc

Mystic Seaport Museum, Inc., G. W. Blunt White Library (1964)

### **New Britain**

Central Connecticut State University Elihu Burritt Library (1973)

### New Haven

Southern Connecticut State University Hilton C. Buley Library (1968) Yale Law Library (1981) Yale University Seeley G. Mudd Library (1859)

### **New London**

Connecticut College C. E. Shain Library (1926) U.S. Coast Guard Academy Library (1939)

#### Stamford

Ferguson Library (1973)

#### Storrs

University of Connecticut Homer Babbidge Library (1907)

# Waterbury

Post College Traurig Library and Learning Resources Center (1977) Silas Bronson Public Library (1869)

# West Haven

University of New Haven Marvin K. Peterson Library (1971)

### **DELAWARE**

#### Dover

State Law Library in Kent County (unknown)

# Georgetown

Delaware Technical and Community College Southern Campus Library (1968)

## Newark

University of Delaware Library (1907)

### Wilmington

Widerne University School of Law Library (1976)

### DISTRICT OF COLUMBIA

# Washington

Administrative Conference of the United States Library (1972) Advisory Commission on Intergovernmental Relations Library (1977) American University Washington College of Law Library (1983) Catholic University of America Robert J. White Law Library (1979)

Comptroller of the Currency Library (1986)

Pentagon Library (1969)

Department of Commerce Library (1955)

Department of Education (1988)

Department of Health and Human Services Library and Information Center (1954)

Department of Housing and Urban Development Library (1969)

Department of the Interior Natural Resources Library (1895) Department of Justice Main Library (1895) Department of Labor Library (1976)

Department of the Navy Library (1895) Department of State Library (1895) Department of State Law Library (1966)

Department of Transportation Main Library (1982)

Department of Transportation, U.S. Coast Guard Law Library (1982)

Department of Veteran's Affairs Library (1967) Department of the Treasury Library (1895) District of Columbia Court of Appeals Library (1981)

District of Columbia Public Library (1943)

Equal Employment Opportunity Commission Library (1984) Executive Office of the President, Library & Information Service Division (1965)

Federal Deposit Insurance Corporation Library (1972) Federal Election Commission Law Library (1975) Federal Energy Regulatory Commission Library (1983)

Federal Mine Safety & Health Review Commission Library (1979) Federal Reserve System Board of Governors Research Library

Federal Reserve System Law Library (1976)

General Accounting Office Office of Library Services (1974)

General Services Administration Library (1975)

Georgetown University Library (1969)

Georgetown University Law Center Edward Bennett Williams Library (1978)

George Washington University Melvin Gelman Library (1983) George Washington University National Law Center Jacob Burns Law

Library (1978) Library of Congress Congressional Research Service (1978)

Library of Congress Serial and Government Publications (1977) Merit Systems Protection Board Library (1979)

National Defense University Library (1895)
Pension Benefit Guaranty Corporation Legal Dept. Library (1984)

U.S. Court of Appeals Judges' Library (1975)
U.S. Court of Appeals for the Federal Circuit Library (1986)

U.S. Information Agency Library (1984)

U.S. Office of Personnel Management Library (1963)

U.S. Postal Service Library (1895) U.S. Senate Library (1979) U.S. Supreme Court Library (1978)

University of the District of Columbia Library Learning Resources Division (1970)

Veterans' Administration Central Office Library (1967)

#### **FLORIDA**

### **Boca Raton**

Florida Atlantic University S. E. Wimberly Library (1963)

Casselberry

Seminole County Public Library (1989)

**Coral Gables** 

University of Miami Otto G. Richter Library (1939)

**Daytona Beach** 

Volusia County Library Center (1963)

De Land

Stetson University duPont-Ball Library (1887)

Fort Lauderdale

Broward County Main Library (1967) Nova University Law Library (1967)

**Fort Plerce** 

Indian River Community College Library (1975)

Galnesville

University of Florida College of Law Library (1978) University of Florida Libraries (1907) REGIONAL

Jacksonville

Haydon Burns Public Library (1914) Jacksonville University Swisher Library (1962) University of North Florida Thomas G. Carpenter Library (1972)

**Key West** 

Florida Keys Community College Key West Campus Library (1989)

Lakeland

Lakeland Public Library (1928)

Leesburg

Lake-Sumter Community College Library (1963)

Melbourne

Florida Institute of Technology Library (1963)

Mlami

Florida International University Library Tamiami Trail (1970) Miami-Dade Public Library (1952)

North Mlami

Florida International University Bay Vista Campus Library (1977)

**Opa Locka** 

St. Thomas University Library (1977)

Orlando

University of Central Florida Library (1966)

Palatka

Saint Johns River Community College Library (1963)

**Panama City** 

Bay County Public Library (1983)

Pensacola

University of West Florida John C. Pace Library (1966)

**Port Charlotte** 

Charlotte-Glades Library System (1973)

Saint Petersburg

Saint Petersburg Public Library (1965) Stetson University College of Law Charles A. Dana Law Library (1975)

Sarasota

Selby Public Library (1970)

Tallahassee

Florida Agricultural and Mechanical University Coleman Memorial Library (1936)

Florida State University Law Library (1978)

Florida State University Strozier Library (1941) Florida Supreme Court Library (1974)

State Library of Florida (1929)

**Tampa** 

Tampa-Hillsborough County Public Library (1965) University of South Florida Library (1962) University of Tampa Merl Kelce Library (1953)

Winter Park

Rollins College Olin Library (1909)

**GEORGIA** 

Albany

Dougherty County Public Library (1964)

**Americus** 

Georgia Southwestern College James Earl Carter Library (1966)

Athens

University of Georgia Libraries (1907) REGIONAL University of Georgia School of Law Library (1979)

### Atlanta

Atlanta-Fulton Public Library (1880)
Atlanta University Center Robert W. Woodruff Library (1962)
Emory University Law School Library (1968)
Emory University Woodruff Library (1928)
Georgia Institute of Technology Price Gilbert Memorial Library (1963)
Georgia State Law Library (unknown)
Georgia State University William Russell Pullen Library (1970)
Georgia State University College of Law Library (1983)
U.S. Court of Appeals 11th Circuit Library (1980)

# Augusta

Augusta College Reese Library (1962) Medical College of Georgia Library (1986)

### Brunswick

Brunswick-Glynn County Regional Library (1965)

### Carrollton

West Georgia College Irvine Sullivan Ingram Library (1962)

## Columbus

Columbus College Simon Schwob Memorial Library (1975)

## Dahlonega

North Georgia College Stewart Library (1939)

## **Dalton**

Dalton College Library (1978)

### Macon

Mercer University Stetson Main Library (1964) Mercer University Walter F. George School of Law Library (1978)

#### Marletta

Kennesaw State College Horace W. Sturgis Library (1968)

# Milledgeville

Georgia College Ina Dillard Russell Library (1950)

### Rome

Berry College Memorial Library (1970)

### Savannah

Chatham-Effingham Liberty Regional Library (1857)

### Statesboro

Georgia Southern University Zach S. Henderson Library (1939)

#### Valdosta

Valdosta State College Library (1956)

### **GUAM**

## Agana

Nieves M. Flores Memorial Library (1962)

# Mangllao

University of Guam Robert F. Kennedy Memorial Library (1978)

### HAWAII

#### HIIO

University of Hawaii at Hilo Edwin H. Mookini Library (1962)

#### Honolulu

Hawaii Medical Library Incorporated (1968)
Hawaii State Library (1929)
Municipal Reference & Records Center (1965)
Supreme Court Law Library (1973)
University of Hawaii Hamilton Library (1907) REGIONAL
University of Hawaii William S. Richardson School of Law Library (1978)

## Lale

Joseph F. Smith Library Brigham Young University Hawaii Campus (1964)

### Lihue

Lihue Public Library (1967)

## **Pearl City**

Leeward Community College Library (1967)

### Walluku

Maui Public Library (1962)

### IDAHO

# **Bolse**

Boise Public Library and Information Center (1929) Boise State University Library (1966) Idaho State Law Library (unknown) Idaho State Library (unknown)

## Caldwell

College of Idaho Terteling Library (1930)

### Crawfordsville

Wabash College Lily Library

### Moscow

University of Idaho College of Law Library (1978) University of Idaho Library (1907) REGIONAL

### Nampa

Northwest Nazarene College John E. Riley Library (1984)

#### **Pocatello**

Idaho State University Eli Oboler Library (1908)

## Rexburg

Davis O. McKay Library (1946)

### **Twin Falls**

College of Southern Idaho Library (1970)

### ILLINOIS

## **BloomIngton**

Illinois Wesleyan University, Sheean Library (1964)

## Carbondale

Southern Illinois University at Carbondale Morris Library (1932) Southern Illinois University School of Law Library (1978)

### Carlinville

Blackburn College Lumpkin Library (1954)

# Carterville

Shawnee Library System (1971)

Chicago Public Library (1876)

University of Chicago Library (1897)

# Champalgn

University of Illinois Law Library (1965)

### Charleston

Eastern Illinois University Booth Library (1962)

### Chicago

Chicago State University Paul and Emily Douglas Library (1954)
DePaul University Law Library (1979)
Field Museum of Natural History Library (1963)
Illinois Institute of Technology Chicago-Kent College of Law Library (1978)
Illinois Institute of Technology Paul V. Galvin Library (1982)
John Marshall Law School Library (1981)
Loyola University of Chicago E. M. Cudahy Memorial Library (1966)
Loyola University School of Law Library (1979)
Northeastern Illinois University Ronald Williams Library (1961)
Northwestern University School of Law Library (1978)
University of Chicago Law Library (1964)

University of Illinois at Chicago Library (1957) William J. Campbell Library of the U.S. Courts (1979)

#### Decatur

Decatur Public Library (1954)

### De Kalb

Northern Illinois University Founders' Memorial Library (1960) Northern Illinois University College of Law Library (1978)

## **Des Plaines**

Government Information Center and The Northwest Municipal Conference Oakton Community College Library (1976)

### Edwardsville

Southern Illinois University at Edwardsville Lovejoy Memorial Library (1959)

#### Elsah

Principia College Marshall Brooks Library (1957)

### **Evanston**

Northwestern University Library (1876)

### Freeport

Freeport Public Library (1905)

#### Galesburg

Galesburg Public Library (1896)

# **Jacksonville**

MacMurray College Henry Pfeiffer Library (1929)

## Kankakee

Olivet Nazarene University Bonner Library and Learning Center (1946)

### Lake Forest

Lake Forest College Donnelley Library (1962)

# Lebanon

McKendree College Holman Library (1968)

#### Lisle

Illinois Benedictine College Theodore F. Lownik Library (1911)

## Macomb

Western Illinois University Government Publications & Legal Reference Library (1962)

#### Moline

Black Hawk College Learning Resources Center (1970)

Monmouth

Monmouth College Hewes Library (1860)

**Mount Carmel** 

Wabash Valley College Bauer Media Center (1975)

**Mount Prospect** 

Mount Prospect Public Library (1977)

Normal

Illinois State University Milner Library (1877)

Oak Park

Oak Park Public Library (1963)

Oglesby

Illinois Valley Community College Jacobs Memorial Library (1976)

Palos Hills

Moraine Valley Community College Learning Resources Center (1972)

Peorla

Cullom-Davis Library (1963) Peoria Public Library (1883)

**River Forest** 

Rosary College Rebecca Crown Library (1966)

Rockford

Rockford Public Library (1895)

Romeoville

Lewis University Library (1952)

South Holland

South Suburban College Learning Resources Center

Springfield

Illinois State Library (unknown) REGIONAL

Streamwood

Poplar Creek Public Library (1980)

**University Park** 

Governors' State University Library (1974)

Urbana

University of Illinois Documents Library (1907)

Wheaton

Wheaton College Buswell Memorial Library (1964)

Woodstock

Woodstock Public Library (1963)

INDIANA

Anderson

Anderson College Charles E. Wilson Library (1959)

Anderson Public Library (1983)

**Bioomington** 

Indiana University Library (1881) Indiana University Law Library (1978)

Crawfordsville

Wabash College Lilly Library (1906)

Evansville

Evansville and Vanderburgh County Public Library (1928)

University of Southern Indiana Library Services (1969)

**Fort Wayne** 

Allen County Public Library (1896) Indiana University-Purdue University at Fort Wayne (1965)

Franklin

Franklin College Library (1976)

Gary

Gary Public Library (1943)

Indiana University Northwest Library (1966)

Greencastle

De Pauw University Roy O. West Library (1879)

Hammond

Hammond Public Library (1964)

Hanover

Hanover College Duggan Library (1892)

Huntington

Huntington College Richlyn Library (1964)

indianapolis

Butler University Irwin Library (1965) Indianapolis-Marion County Public Library (1906) Indiana State Library (unknown) REGIONAL Indiana Supreme Court Law Library (1975)

Indiana University School of Law Library (1967) Indiana University-Purdue University Library (1979)

#### Kokomo

Indiana University at Kokomo Learning Resource Center (1969)

### Muncle

Ball State University Alexander M. Bracken Library (1959) Muncie Public Library (1906)

## **New Albany**

Indiana University Southeast Library (1965)

### **Notre Dame**

Notre Dame Law School Kresge Law Library (1985) University of Notre Dame Hesburgh Library (1883)

#### Rensselaer

Saint Joseph's College Library (1964)

### Richmond

Earlham College Lilly Library (1964) Morrison-Reeves Library (1906)

## South Bend

Indiana University at South Bend Franklin D. Schurz Library (1965)

#### **Terre Haute**

Indiana State University Cunningham Memorial Library (1906)

### Valparaiso

Valparaiso University Moellering Memorial Library (1930) Valparaiso University Law Library (1978)

# **West Lafayette**

Purdue University Libraries (1907)

## **IOWA**

#### Ames

Iowa State University Parks Library (1907)

### Cedar Falls

University of Northern Iowa Donald O. Rod Library (1946)

## Cedar Rapids

Cedar Rapids Public Library (1986)

# **Council Bluffs**

Free Public Library (1885)
Iowa Western Community College Herbert Hoover Library (1972)

### Davenport

Davenport Public Library (1973)

#### Des Moines

Drake University Cowles Library (1966) Drake University Law Library (1972) Public Library of Des Moines (1888) State Library of Iowa (unknown)

# **Dubuque**

Carnegie-Stout Public Library (unknown) Loras College Wahlert Memorial Library (1967)

### **Fayette**

Upper Iowa University Henderson-Wilder Library (1974)

#### Grinnell

Grinnell College Burling Library (1874)

## **Iowa City**

University of Iowa College of Law Library (1968) University of Iowa Libraries (1884) REGIONAL

#### Lamoni

Graceland College Frederick Madison Smith Library (1927)

### Mason City

North Iowa Area Community College Library (1976)

### **Mount Vernon**

Cornell College Russell D. Cole Library (1896)

## **Orange City**

Northwestern College Ramaker Library (1970)

# Sloux City

Sioux City Public Library (1894)

# KANSAS

### Atchison

Benedictine College Library (1965)

# **Baidwin City**

Baker University Collins Library (1908)

#### Colby

Colby Community College H. F. Davis Memorial Library (1968)

## **Emporla**

Emporia State University William Allen White Library (1909)

## Hays

Fort Hays State University Forsyth Library (1926)

#### Hutchinson

Hutchinson Public Library (1963)

#### Lawrence

University of Kansas Law Library (1971) University of Kansas Map Library (1869) REGIONAL

### Manhattan

Kansas State University Farrell Library (1907)

### **Pittsburg**

Pittsburg State University Leonard H. Axe Library (1952)

### Salina

Kansas Weslevan University Memorial Library (1930)

#### Shawnee Mission

Johnson County Library (1979)

# Topeka

Kansas State Historical Society Library (1877) Kansas State Library (unknown) Kansas Supreme Court Law Library (1975) Washburn University of Topeka Law Library (1971)

## Wichita

Wichita State University Ablah Library (1901)

#### KENTUCKY

#### **Ashland**

Ashland Community College Library (1946)

## Barbourville

Union College Abigail E. Weeks Memorial Library (1958)

## **Bowling Green**

Western Kentucky University Helm-Cravens Library (1934)

### Columbia

Lindsey Wilson College Katie Murrell Library (1987)

#### Crestview Hills

Thomas More College Library (1970)

### Danville

Centre College Grace Doherty Library (1884)

### Frankfort

Kentucky Department of Libraries and Archives (1967) Kentucky State Law Library (unknown) Kentucky State University Blazer Library (1972)

#### Hazard

Hazard Community College Library (1988)

# **Highland Heights**

Northern Kentucky University W. Frank Steely Library (1973)

# Lexington

University of Kentucky Law Library (1968) University of Kentucky Libraries (1907) REGIONAL

### Louisville

Louisville Free Public Library (1904) University of Louisville Ekstrom Library (1925) University of Louisville Law Library (1975)

#### Morehead

Morehead State University Camden-Carroll Library (1955)

### Murray

Murray State University Waterfield Library (1924)

## Owensboro

Kentucky-Wesleyan College Library Learning Center (1966)

### Richmond

Eastern Kentucky University John Grant Crabbe Library (1966)

### Williamsburg

Cumberland College Norma Perkins Hagan (1988)

## LOUISIANA

# **Baton Rouge**

Louisiana State Library (1976)
Louisiana State University Middleton Library (1907) REGIONAL
Louisiana State University Paul M. Hebert Law Center Library (1929)
Southern University John B. Cade Library (1952)
Southern University Law School Library (1979)

#### Eunice

Louisiana State University at Eunice LeDoux Library (1969)

## Hammond

Southeastern Louisiana University Sims Memorial Library (1966)

## Lafayette

University of Southwestern Louisiana Dupre Library (1938)

#### Lake Charles

McNeese State University Lether E. Frazar Memorial Library (1941)

## Monroe

Northeast Louisiana University Sandel Library (1963)

#### **Natchitoches**

Northwestern State University Watson Memorial Library (1887)

### **New Orleans**

Law Library of Louisiana (unknown)
Loyola University Government Documents Library (1942)
Loyola University Law Library (1978)
New Orleans Public Library (1883)
Our Lady of Holy Cross College Library (1968)
Southern University in New Orleans Leonard S. Washington Memorial
Library (1962)

Tulane University Law Library (1976)
Tulane University Howard-Tilton Memorial Library (1942)
U.S. Court of Appeals 5th Circuit Library (1973)

University of New Orleans Earl K. Long Library (1963)

## **Pineville**

Louisiana College Richard W. Norton Memorial Library (1969)

### Ruston

Louisiana Technical University Prescott Memorial Library (1896) REGIONAL

# Shreveport

Louisiana State University at Shreveport Library (1967) Shreve Memorial Library (1923)

## **Thibodaux**

Nicholls State University Ellender Memorial Library (1962)

### MAINE

## Augusta

Maine Law and Legislative Reference Library (1973) Maine State Library (unknown)

### Bangor

Bangor Public Library (1884)

#### Brunswick

Bowdoin College Library (1884)

#### Castine

Maine Maritime Academy Nutting Memorial Library (1969)

#### Lewiston

Bates College George and Helen Ladd Library (1883)

### Orono

University of Maine Raymond H. Fogler Library (1907) REGIONAL

### **Portland**

Portland Public Library (1884) University of Maine School of Law Garbrecht Law Library (1964)

# Presque Isle

University of Maine at Presque Isle Library/Learning Resources Center (1979)

#### Sanford

Louis B. Goodall Memorial Library (1984)

### Waterville

Colby College Miller Library (1884)

### MARYLAND

# Annapolis

Maryland State Law Library (unknown) U.S. Naval Academy Nimitz Library (1895)

## **Baitimore**

Enoch Pratt Free Library (1887)
Johns Hopkins University Milton S. Eisenhower Library (1882)
Morgan State University Soper Library (1940)
University of Baltimore Langsdale Library (1973)
University of Baltimore Law Library (1980)
University of Maryland School of Law Marshall Law Library (1969)
U.S. Court of Appeals 4th Circuit Library (1982)

#### Bel Alr

Harford Community College Library (1967)

#### Beltsville

Department of Agriculture National Agricultural Library (1895)

### Bethesda

Department of Health and Human Services National Library of Medicine (1978)
Uniformed Services University of Health Sciences Learning Resource Center (1983)

### Catonsville

University of Maryland, Baltimore County Albin O. Kuhn Library & Gallery (1971)

## Chestertown

Washington College Clifton M. Miller Library (1891)

# College Park

University of Maryland Hornbake Library (1925) REGIONAL

### Cumberland

Allegany Community College Library (1974)

## Frostburg

Frostburg State University Library (1967)

#### **Patuxent River**

Patuxent River Central Library (1968)

#### Rockville

Montgomery County Department of Public Libraries (1951)

## Sallsbury

Salisbury State College Blackwell Library (1965)

### Towson

Goucher College Julia Rogers Library (1966) Towson State University Cook Library (1979)

#### Westminster

Western Maryland College Hoover Library (1886)

## **MASSACHUSETTS**

### **Amherst**

Amherst College Library (1884) University of Massachusetts University Library (1907)

## **Boston**

Boston Athenaeum Library (unknown)
Boston Public Library (1859) REGIONAL
Boston University School of Law (1979)
Northeastern University Snell Library (1962)
State Library of Massachusetts (unknown)
Suffolk University Law Library (1979)
Supreme Judicial Court Social Law Library (1979)
U.S. Court of Appeals First Circuit Library (1978)

### Brookline

Public Library of Brookline (1925)

# Cambridge

Harvard College Library (1860) Harvard Law School Library (1981) Massachusetts Institute of Technology Library (1946)

### Chestnut Hill

Boston College Thomas P. O'Neill Jr., Library (1963)

## Chicopee

College of Our Lady of the Elms Alumnae Library (1969)

#### Lowell

University of Lowell O'Leary Library (1952)

#### Medford

Tufts University Wessel Library (1899)

### Milton

Curry College Levin Library (1972)

#### **New Bedford**

New Bedford Free Public Library (1858)

### **Newton Centre**

Boston College Law School Library (1979)

#### North Dartmouth

Southeastern Massachusetts University Library (1965)

### North Easton

Stonehill College Cushing-Martin Library (1962)

# Springfield

Springfield City Library (1966) Western New England College School of Law Library (1978)

## Waltham

Brandeis University Library (1965) Waltham Public Library (1982)

## Wellesley

Wellesley College Margaret Clapp Library (1943)

#### Wenham

Gordon College Jenks Learning Resource Center (1963)

### Williamstown

Williams College Sawyer Library (unknown)

#### Worcester

American Antiquarian Society Library (1814) University of Massachusetts Medical Center Library (1972) Worcester Public Library (1859)

### **MICHIGAN**

## **Albion**

Albion College Stockwell-Mudd Library (1966)

### Allendale

Grand Valley State College Zumberge Library (1963)

### Alma

Alma College Library (1963)

#### Ann Arbor

University of Michigan Harlan Hatcher Graduate Library (1884) University of Michigan Law Library (1978)

### **Benton Harbor**

Benton Harbor Public Library (1907)

## **Bloomfleld Hills**

Cranbrook Institute of Science Library (1940)

### Dearborn

Henry Ford Centennial Library (1969) Henry Ford Community College Library (1957)

### Detroit

Detroit College of Law Library (1979)
Detroit Public Library (1868) REGIONAL
Marygrove College Library (1965)
Mercy College of Detroit Library (1965)
University of Detroit Library (1884)
University of Detroit School of Law Library (1978)
Wayne State University Purdy/Kresge Library (1937)
Wayne State University Arthur Neef Law Library (1971)

# Dowaglac

Southwestern Michigan College Matthews Library (1971)

## East Lansing

Michigan State University Government Documents Library (1907)

# **Farmington Hills**

Oakland Community College Martin L. King Learning Resources Center (1968)

### Flint

Flint Public Library (1967) University of Michigan-Flint Library (1977)

# **Grand Rapids**

Calvin College & Seminary Library (1967) Grand Rapids Public Library (1876)

# Houghton

Michigan Technological University J. Robert Van Pelt Library (1876)

## **Jackson**

Jackson District Library (1965)

### Kalamazoo

Kalamazoo Public Library (1907) Western Michigan University Dwight B. Waldo Library (1963)

## Lansing

Library of Michigan (unknown) REGIONAL Thomas M. Cooley Law School Library (1978)

### Livonia

Livonia Public Library (1987) Schoolcraft College Library (1962)

# **Madison Heights**

Madison Heights Public Library (1982)

#### Marquette

Northern Michigan University Lydia M. Olson Library (1963)

#### Monroe

Monroe County Library System (1974)

### **Mount Clemens**

Macomb County Library (1968)

### **Mount Pleasant**

Central Michigan University Charles V. Park Library (1958)

#### Muskegon

Hackley Public Library (1894)

# Petoskev

North Central Michigan College Library (1962)

### Port Huron

Saint Clair County Library (1876)

Rochester

Oakland University Kresge Library (1964)

Royal Oak

Royal Oak Public Library (1984)

Saginaw

Hoyt Public Library (1890)

Sault Ste. Marie

Lake Superior State University Kenneth Shouldice Library (1982)

**Traverse City** 

Northwestern Michigan College Mark and Helen Osterlin Library (1964)

**University Center** 

Delta College Library (1963)

Warren

Warren Public Library Arthur J. Miller Branch (1973)

**Ypsilanti** 

Eastern Michigan University Library (1965)

**MICRONESIA** 

East Caroline Islands

Community College of Micronesia Library (1982)

**MINNESOTA** 

Bemidji

Bernidji State University A.C. Clark Library (1963)

Blaine

Anoka County Library (1971)

Collegeville

Saint John's University Alcuin Library (1954)

**Cottage Grove** 

Washington County Library-Park Grove Branch (1983)

Duluth

Duluth Public Library (1909) University of Minnesota Duluth Library (1984)

Eagan

Dakota County Library-Westcott Branch (1983)

Edina

Southdale-Hennepin Area Library (1971)

Mankato

Mankato State University Memorial Library (1962)

Marshall

Southwest State University Library (1986)

**Minneapolis** 

Minneapolis Public Library (1893) University of Minnesota Law School Library (1978) University of Minnesota Wilson Library (1907) REGIONAL

Moorhead

Moorhead State University Livingston Lord Library (1956)

Morris

University of Minnesota, Morris, Rodney A. Briggs Library (1963)

Northfield

Carleton College Library (1930) Saint Olaf College Rolvaag Memorial Library (1930)

Saint Cloud

Saint Cloud State University, Learning Rescources Center (1962)

Saint Paul

Hamline University School of Law Library (1978)
Minnesota Historical Society Library (1867)
Minnesota State Law Library (unknown)
Saint Paul Public Library (1914)
University of Minnesota Saint Paul Campus Library (1974)
William Mitchell College of Law Library (1979)

Saint Peter

Gustavus Adolphus College Fake Bernadette Memorial Library (1941)

Winona

Winona State University Maxwell Library (1969)

### MISSISSIPPI

### Cleveland

Delta State University W. B. Roberts Library (1975)

## Columbus

Mississippi University for Women John Clayton Fant Memorial Library (1929)

## Hattlesburg

University of Southern Mississippi Joseph A. Cook Memorial Library (1935)

### Jackson

Jackson State University Henry Thomas Sampson Library (1968) Millsaps College Millsaps-Wilson Library (1963) Mississippi College School of Law Library (1977) Mississippi Library Commission (1947) Mississippi State Law Library (unknown)

#### Lorman

Alcorn State University J. D. Boyd Library (1970)

# Mississippi State

Mississippi State University Mitchell Memorial Library (1907)

### University

University of Mississippi J. D. Williams Library (1883) REGIONAL University of Mississippi James O. Eastland Law Library (1967)

### MISSOURI

### Cape Glrardeau

Southeast Missouri State University Kent Library (1916)

### Columbia

University of Missouri at Columbia Ellis Library (1862) REGIONAL University of Missouri-Columbia Law Library (1978)

## **Fulton**

Westminster College Reeves Library (1875)

### Hilisboro

Jefferson College Library (1984)

## Jefferson City

Lincoln University Inman E. Page Library (1944) Missouri State Library (1963) Missouri Supreme Court Library (unknown)

# Joplin

Missouri Southern State College George A. Spiva Library (1966)

# Kansas City

Kansas City Missouri Public Library (1881)
Rockhurst College Greenlease Library (1917)
University of Missouri at Kansas City General Library (1938)
University of Missouri Kansas City Leon E. Bloch Law Library (1978)

### Kirksville

Northeast Missouri State University Pickler Memorial Library (1966)

## Liberty

William Jewell College Charles F. Curry Library (1900)

# Maryville

Northwest Missouri State University B. D. Owens Library (1982)

#### Rolla

University of Missouri-Rolla Curtis Laws Wilson Library (1907)

#### Saint Charles

Kisker Road Branch Library Lindenwood College Margaret Leggat Butler Library (1973)

# Saint Joseph

River Bluffs Regional Public Library (1891)

#### Saint Louis

Maryville College Library (1976)
Saint Louis County Library (1970)
Saint Louis Public Library (1866)
Saint Louis University Law Library (1967)
Saint Louis University Pius XII Memorial Library (1866)
U.S. Court of Appeals Eighth Circuit Library (1972)
University of Missouri at Saint Louis Thomas Jefferson Library (1966)
Washington University John M. Olin Library (1906)
Washington University Law Library (1978)

# Springfield

Drury College, Walker Library (1874) Southwest Missouri State University Duane G. Meyer Library (1963)

# Warrensburg

Central Missouri State University Ward Edwards Library (1914)

# **MONTANA**

## Billings

Eastern Montana College Library (1958)

## Bozeman

Montana State University Libraries (1907)

### **Butte**

Montana College of Mineral Science and Technology Library (1901)

#### Havre

Northern Montana College Vande Bogart Library (1980)

# Helena

Carroll College Corrette Library (1974) Montana State Library (1966) State Law Library of Montana (1977)

### Missoula

University of Montana Maurene & Mike Mansfield Library (1909) REGIONAL

### **NEBRASKA**

### Blair

C. A. Dana College Dana-LIFE Library (1924)

# Crete

Doane College Perkins Library (1944)

#### Fremont

Midland Lutheran College Luther Library (1924)

## Kearney

Kearney State College Calvin T. Ryan Library (1962)

## Lincoln

Nebraska Library Commission (1972) Nebraska State Library (unknown) University of Nebraska-Lincoln College of Law Library (1981) University of Nebraska-Lincoln D. L. Love Memorial Library (1907) REGIONAL

### Omaha

Creighton University Reinert/Alumni Library (1964) Creighton University School of Law Library (1979) Omaha Public Library W. Dale Clark Library (1880) University of Nebraska at Omaha University Library (1939)

### Scottsbluff

Scottsbluff Public Library (1925)

## Wavne

Wayne State College U.S. Conn Library (1970)

## **NEVADA**

# Carson City

Nevada State Library and Archives (unknown) Nevada Supreme Court Library (1973)

# Las Vegas

Clark County Law Library (1988) Las Vegas-Clark County Library (1974) University of Nevada at Las Vegas James Dickinson Library (1959)

#### Reno

National Judicial College Law Library (1979) Nevada Historical Society Library (1974) University of Nevada-Reno Library (1907) REGIONAL Washoe County Library (1980)

#### **NEW HAMPSHIRE**

### Concord

Franklin Pierce Law Center Library (1973) New Hampshire State Library (unknown)

### Durham

University of New Hampshire Library (1907)

### Hanover

Dartmouth College Library (1884)

## Henniker

New England College Danforth Library (1966)

#### Manchester

Manchester City Library (1884) New Hampshire College H. A. B. Shapiro Memorial Library (1976) Saint Anselm College Geisel Library (1963)

#### Nashua

Nashua Public Library (1971)

## **NEW JERSEY**

# Bayonne

Bayonne Free Public Library (1909)

### **Bioomfield**

Bloomfield Public Library (1965)

# **Bridgeton**

Cumberland County Library (1966)

### Camden

Rutgers University Camden Library (1966) Rutgers University School of Law Library (1979)

#### **Convent Station**

College of Saint Elizabeth Mahoney Library (1938)

## **East Brunswick**

East Brunswick Public Library (1977)

# **East Orange**

East Orange Public Library (1966)

#### Elizabeth

Free Public Library of Elizabeth (1895)

## Glassboro

Glassboro State College Savitz Library (1963)

# Hackensack

Johnson Free Public Library (1966)

## irvington

Irvington Public Library (1966)

## **Jersey City**

Jersey City Public Library (1879) Jersey City State College Forrest A. Irwin Library (1963)

#### Lawrenceville

Rider College Franklin F. Moore Library (1975)

#### Madison

Drew University Library (1939)

#### Mahwah

Ramapo College Library (1971)

## **Mount Holly**

**Burlington County Library (1966)** 

#### **New Brunswick**

Rutgers University Alexander Library (1907)

# Newark

Newark Public Library (1906) REGIONAL Rutgers University John Cotton Dana Library (1966) Rutgers University Law Library (1979) Seton Hall University Law Library (1979)

#### Newton

Sussex County Library (1986)

#### **Passaic**

Passaic Public Library (1964)

## **Phillipsburg**

Phillipsburg Free Public Library (1976)

#### Plainfield

Plainfield Public Library (1971)

### **Pomona**

Stockton State College Library (1972)

#### Princeton

Princeton University Firestone Library (1884)

### Randolph

County College of Morris Sherman H. Masten Learning Resource Center (1975)

## Rutherford

Fairleigh Dickinson University Messler Library (1953)

## Shrewsbury

Monmouth County Library (1968)

## South Orange

Seton Hall University Library (1947)

# Teaneck

Fairleigh Dickinson University Weiner Library (1963)

### **Toms River**

Ocean County College Learning Resources Center (1966)

### **Trenton**

New Jersey State Library (unknown) Trenton Free Public Library (1902)

# Unlon

Kean College of New Jersey Nancy Thompson Library (1971)

# **Upper Montclair**

Montclair State College Harry A. Sprague Library (1967)

## Wayne

Wayne Public Library (1972)

# West Long Branch

Monmouth College Guggenheim Memorial Library (1963)

# Woodbridge

Woodbridge Public Library (1965)

### **NEW MEXICO**

### Albuquerque

University of New Mexico Medical Center Library (1973)
University of New Mexico School of Law Library (1973)
University of New Mexico General Library (1896) REGIONAL

### Hobbs

New Mexico Junior College Pannell Library (1969)

# Las Cruces

New Mexico State University Library (1907)

### Las Vegas

New Mexico Highlands University Donnelly Library (1913)

### **Portales**

Eastern New Mexico University Golden Library (1962)

### Santa Fe

New Mexico State Library (1960) REGIONAL New Mexico Supreme Court Law Library (unknown)

# Sliver City

Western New Mexico University Miller Library (1972)

#### Socorro

New Mexico Institute of Mining & Technology Martin Speare Memorial Library (1984)

### **NEW YORK**

# **Albany**

Albany Law School Schaffer Law Library (1979) New York State Library (unknown) REGIONAL State University of New York at Albany University Library (1964)

### Auburn

Seymour Library (1972)

## Bellport

East Islip Public Library (1973)

# Binghamton

State University of New York at Binghamton Glenn G. Bartle Library (1962)

# **Brockport**

State University of New York at Brockport Drake Memorial Library (1967)

### **Bronx**

Fordham University Library (1937)
Lehman College Library (1967)
New York Public Library (1973)
State University of New York Maritime College Stephen B. Luce Library (1947)

### **Bronxville**

Sarah Lawrence College Esther Raushenbush Library (1969)

### Brooklyn

Brooklyn College Library (1936)
Brooklyn Law School Library (1974)
Brooklyn Public Library Business Library (1984)
Brooklyn Public Library (1908)
Pratt Institute Library (1891)
State University of New York Health Center at Brooklyn Library (1958)

#### Buffalo

Buffalo and Erie County Public Library (1895)
State University of New York at Buffalo Charles B. Sears Law Library (1978)
State University of New York at Buffalo Lockwood Memorial Library (1963)

## Canton

Saint Lawrence University Owen D. Young Library (1920)

## Corning

Coming Community College Arthur A. Houghton Jr. Library (1963)

### Cortland

State University of New York at Cortland Memorial Library (1964)

### Delhi

State University College of Technology Resnick Library (1970)

#### **Elmira**

Elmira College Gannett Tripp Learning Center (1956)

## **Farmingdale**

State University of New York at Farmingdale Greenley Library (1917)

## Flushing

CUNY Law School at Queens College CUNY Law Library (1983) Queens College Benjamin S. Rosenthal Library (1939)

# **Garden City**

Adelphi University Swirbul Library (1966)

#### Geneseo

State University of New York at Geneseo Milne Library (1967)

# Greenvale

Long Island University B. Davis Schwartz Memorial Library (1964)

# Hamilton

Colgate University, Everett Needham Case Library (1902)

## Hempstead

Hofstra University Library (1964) Hofstra University School of Law Library (1979)

### Huntington

Touro College Jacob D. Fuchsberg Law Center Library (1985)

## Ithaca

Comell University Library (1907) Comell Law Library (1978) Comell University Albert R. Mann Library (1943)

### Jamaica

Queens Borough Public Library (1926) Saint John's University Library (1956) Saint John's University School of Law Library (1978)

## Kings Point

U.S. Merchant Marine Academy Schuyler Otis Bland Library (1962)

## Long Island City

Fiorello H. LaGuardia Community College Library (1981)

### Middletown

Thrall Library (1986)

### **Mount Vernon**

Mount Vernon Public Library (1962)

#### **New Paltz**

State University College at New Paltz Sojourner Truth Library (1965)

## **New York City**

City College of City University of New York Cohen Library (1884)

College of Insurance Library (1965)

Columbia University Libraries (1882)

Columbia University School of Law Library (1981)

Cooper Union for the Advancement of Science and Arts Library (1930)

Fordham Law School Library (1987)

Medical Library Center of New York (1976)

New York Law Institute Library (1909) New York Law School Library (1979)

New York Public Library Astor Branch (1907)

New York Public Library Lenox Branch (1884)

New York University Law Library (1974)

New York University Elmer Holmes Bobst Library (1967)

U.S. Court of Appeals Second Circuit Library (1976)

Yeshiva University Chutick Law Library Cardozo School of Law (1979)

Yeshiva University Pollack Library (1979)

# Newburgh

Newburgh Free Library (1909)

## Niagara Falls

Niagara Falls Public Library (1976)

### **Oakdale**

Dowling College Library (1965)

# Oneonta

State University College at Onenonta James M. Milne Library (1966)

## Oswego

State University of New York at Oswego Penfield Library (1966)

# **Plattsburgh**

State University College at Plattsburgh Benjamin F. Feinberg Library (1967)

### Potsdam

Clarkson University Hamet Call Burnap Memorial Library (1938) State University College of New York at Potsdam Frederick W. Crumb Memorial Library (1964)

# Poughkeepsle

Vassar College Library (1943)

### **Purchase**

State University of New York at Purchase Library (1969)

## Rochester

Rochester Public Library (1963) University of Rochester Rush Rhees Library (1880)

#### Saint Bonaventure

Saint Bonaventure University Friedsam Memorial Library (1938)

# Saratoga Springs

Skidmore College Library (1964)

## Schenectady

Union College Schaffer Library (1901)

# Southampton

Long Island University Southhampton Campus Library (1973)

#### Sparkili

St. Thomas Aguinas College Lougheed Library (1984)

# Staten Island

Wagner College Horrmann Library (1953)

# Stony Brook

State University of New York at Stony Brook Main Library (1963)

### Syracuse

Onondaga County Public Library (1978) Syracuse University Library (1878) Syracuse University College of Law H. Douglas Barclay Law Library (1978)

# Trov

Troy Public Library (1869)

### Uniondale

Nassau Library System (1965)

### Utica

Utica Public Library (1885) SUNY Institute of Technology Library (1977)

### **West Point**

U.S. Military Academy Library (unknown)

### White Plains

Pace University Law Library (1978)

## **Yonkers**

Yonkers Public Library Getty Square Branch (1910)

# Yorktown Heights

Mercy College Library (1976)

## **NORTH CAROLINA**

#### Asheville

University of North Carolina at Asheville D. Hiden Ramsey Library (1965)

# **Bolling Springs**

Gardner-Webb College Dover Memorial Library (1974)

### **Boone**

Appalachian State University Carol Grotnes Belk Library (1963)

#### **Bules Creek**

Campbell University Carrie Rich Memorial Library (1965)

## Chapel Hill

University of North Carolina at Chapel Hill Davis Library (1884) REGIONAL University of North Carolina at Chapel Hill Law Library (1978)

# Charlotte

Public Library of Charlotte and Mecklenburg County (1964) Queens College Everett Library (1927) University of North Carolina at Charlotte Atkins Library (1964)

# Cullowhee

Western Carolina University Hunter Library (1953)

#### Davidson

Davidson College Library (1893)

### Durham

Duke University School of Law Library (1978)
Duke University William R. Perkins Library (1890)
North Carolina Central University Law School Library (1979)
North Carolina Central University James E. Shepard Memorial Library (1973)

## **Elon College**

Elon College Iris Holt McEwen Library (1971)

# **Fayetteville**

Fayetteville State University Charles W. Chesnutt Library (1971)

## Greensboro

North Carolina Agricultural and Technical State University F. D. Bluford Library (1937) University of North Carolina at Greensboro Walter Clinton Jackson Library (1963)

#### Greenville

East Carolina University J. Y. Joyner Library (1951)

## Laurinburg

Saint Andrews Presbytenian College DeTamble Library (1969)

## Lexington

Davidson County Public Library (1971)

#### **Mount Olive**

Mount Olive College Moye Library (1971)

### **Pembroke**

Pembroke State University Mary H. Livermore Library (1956)

### Raleigh

Department of Cultural Resources Division of State Library (unknown) North Carolina State University D. H. Hill Library (1923) North Carolina Supreme Court Library (1972)

## **Rocky Mount**

North Carolina Wesleyan College Library (1969)

## Sallsbury

Catawba College Library (1925)

### Wilmington

University of North Carolina at Wilmington William M. Randall Library (1965)

## Wilson

Barton College Hackney Library (1930)

#### Winston-Salem

Forsyth County Public Library (1954) Wake Forest University School of Law Library (1902)

### **NORTH DAKOTA**

#### **Blsmarck**

North Dakota State Library (1971)
North Dakota Supreme Court Law Library (unknown)
State Historical Society of North Dakota State Archives & Historical Research Library (1907)
Veterans' Memorial Public Library (1967)

#### Dickinson

Dickinson State University Stoxen Library (1968)

## Fargo

Fargo Public Library (1964) North Dakota State University Library (1907) REGIONAL

### **Grand Forks**

University of North Dakota Chester Fritz Library (1890)

### Minot

Minot State University Memorial Library (1925)

## **Valley City**

Valley City State University Allen Memorial Library (1913)

## NORTHERN MARIANA ISLANDS

## Salpan

Northern Marianas College Olympio T. Borja Memorial Library (1988)

# OHIO

## Ada

Ohio Northern University J. P. Taggart Law Library (1965)

#### Akron

Akron-Summit County Public Library (1952) University of Akron Bierce Library (1963) University of Akron School of Law Library (1978)

## Alllance

Mount Union College Library (1888)

### **Ashland**

Ashland University Library (1938)

#### Athens

Ohio University Alden Library (1886)

### Batavla

University of Cincinnati Clermont College Library (1973)

### Bluffton

Bluffton College Musselman Library (1951)

# **Bowling Green**

Bowling Green State University Jerome Library (1933)

#### Canton

Malone College Everett L. Cattel Library (1970)

#### Chardon

Chardon Public Library (1971)

#### Cincinnati

Public Library of Cincinnati and Hamilton County (1884) University of Cincinnati Langsam Library (1929) University of Cincinnati College of Law Marx Law Library (1978) U.S. Court of Appeals 6th Circuit Library (1986)

### Cleveland

Case Western Reserve University Freiberger Library (1913)
Case Western Reserve University School of Law Library (1979)
Cleveland Public Library (1886)
Cleveland State University Cleveland-Marshall College of Law,
Joseph W. Bartunek III Law Library (1978)
Cleveland State University Library (1966)
Municipal Reference Library (1970)

### Cleveland Heights

Cleveland Heights-University Heights Public Library (1970)

### Columbus

Capital University Law School Library (1980)
Capital University Library (1968)
Columbus Metropolitan Library (1885)
Ohio State University College of Law Library (1984)
Ohio State University Libraries (1907)
Ohio Supreme Court Law Library (1973)
State Library of Ohio (unknown) REGIONAL

# Dayton

Dayton and Montgomery County Public Library (1909) University of Dayton Roesch Library (1969) Wright State University Library (1965)

### Delaware

Ohio Wesleyan University L. A. Beeghly Library (1845)

## Elvria

Elyria Public Library (1966)

## **Findiay**

Findlay University of Shafer Library (1969)

### Gambler

Kenyon College Library (1873)

#### Granville

Denison University Libraries William H. Doane Library (1884)

#### Hiram

Hiram College Teachout-Price Memorial Library (1874)

## Kent

Kent State University Libraries (1962)

### Marletta

Marietta College Dawes Memorial Library (1884)

## Marlon

Marion Public Library (1979)

### Middletown

Miami University Middletown Gardner-Harvey Library (1970)

## **New Concord**

Muskingum College Library (1966)

## Oberiln

Oberlin College Library (1858)

## Oxford

Miami University Libraries King Library (1909)

### **Portsmouth**

Shawnee State University Library (1987)

### Rlo Grande

University of Rio Grande Jeanette Albiez Davis Library (1966)

# Springfield

Clark County Public Library (1884)

## Steubenville

Franciscan University of Steubenville John Paul II Library (1971) Public Library of Steubenville and Jefferson County (1950)

#### Tiffin

Heidelberg College Beeghly Library (1964)

### Toledo

Toledo-Lucus County Public Library (1884) University of Toledo College of Law Library (1981) University of Toledo Library (1963)

# **University Heights**

John Carroll University Grasselli Library (1963)

### Westerville

Otterbein College Courtright Memorial Library (1967)

## Wilmington

Wilmington College S. Arthur Watson Library (1986)

### Wooster

College of Wooster Andrews Library (1966)

## WorthIngton

Worthington Public Library (1984)

## Youngstown

Public Library of Youngstown and Mahoning County (1923) Youngstown State University William F. Maag Library (1971)

# **OKLAHOMA**

### Ada

East Central Oklahoma State University Linscheid Library (1914)

#### Alva

Northwestern Oklahoma State University J. W. Martin Library (1907)

## Bethany

Southern Nazarene University R. T. Williams Learning Resources Center (1971)

### Durant

Southeastern Oklahoma State University Henry G. Bennett Memorial Library (1929)

### **Edmond**

Central State University Library (1934)

#### Enld

Public Library of Enid and Garfield County (1908)

## Langston

Langston University G. Lamar Harrison Library (1941)

#### Lawton

Lawton Public Library (1987)

#### Norman

University of Oklahoma Libraries Bizzell Memorial Library (1893) University of Oklahoma Law Library (1978)

# Oklahoma City

Metropolitan Library System Main Library (1974) Oklahoma City University Dulaney Browne Library (1963) Oklahoma Department of Libraries (1893) REGIONAL

#### Shawnee

Oklahoma Baptist University Library (1933)

### Stillwater

Oklahoma State University Edmon Low Library (1907) REGIONAL

## Tahlequah

Northeastern Oklahoma State University John Vaughan Library (1923)

### Tulsa

Tulsa City-County Library System (1963) University of Tulsa College of Law Library (1979) University of Tulsa McFarlin Library (1929)

#### Weatherford

Southwestern Oklahoma State University Al Harris Library (1958)

### **OREGON**

#### **Ashland**

Southern Oregon State College Library (1953)

# Bend

Central Oregon Community College Library/Media Service (1985)

Corvailis

Oregon State University Library (1907)

Eugene

University of Oregon Law Library (1979) University of Oregon Library (1883)

**Forest Grove** 

Pacific University Harvey W. Scott Memorial Library (1897)

Klamath Falls

Oregon Institute of Technology Library (1982)

La Grande

Eastern Oregon State College Walter M. Pierce Library (1954)

McMinnville

Linfield College Northup Library (1965)

Monmouth

Western Oregon State College Library (1967)

Pendleton

Blue Mountain Community College Library (1983)

**Portland** 

Lewis and Clark College Aubrey R. Watzek Library (1967) Multnomah County Portland (1884) Northwestern School of Law Lewis and Clark College Paul L. Boley Law Library (1979) Portland State University Millar Library (1963) REGIONAL

Reed College Library (1912)

U.S Department of Energy Bonneville Power Administration Library (1962)

Salem

Oregon State Library (unknown) Oregon Supreme Court Law Library (1974) Willamette University College of Law Library (1979) Willamette University Main Library (1969)

**PANAMA** 

**Balboa Heights** 

Panama Canal Commission Technical Resources Center

**PENNSYLVANIA** 

Allentown

Muhlenberg College Trexter Library (1939)

Altoona

Altoona Area Public Library (1969)

**Bethel Park** 

Bethel Park Public Library (1980)

Bethlehem

Lehigh University Libraries Linderman Library (1876)

Blue Bell

Montgomery County Community College Learning Resources Center (1975)

**Bradford** 

University of Pittsburgh at Bradford T. Edwards & Tullah Hanley Library (1979)

**Broomali** 

Marple Public Library (1988)

California

California University of Pennsylvania Louis L. Manderino Library (1986)

Carlisle

Dickinson College Boyd Lee Spahr Library (1947) Dickinson School of Law Sheeley-Lee Law Library (1978)

Cheyney

Cheyney University Leslie Pinckney Hill Library (1967)

Collegeville

Ursinus College Myrin Library (1963)

Coraopolls

Robert Morris College Library (1978)

Doylestown

Bucks County Free Library (1970)

East Stroudsburg

East Stroudsburg University Kemp Library (1966)

Erle

Erie County Library System (1897)

Greenville

Thiel College Langenheim Memorial Library (1963)

# Harrisburg

State Library of Pennsylvania (unknown) REGIONAL Widener University Harrisburg Campus School of Law Library

#### Haverford

Haverford College Magill Library (1897)

#### Hazleton

Hazleton Area Public Library (1964)

#### indiana

Indiana University of Pennsylvania Stapleton Library (1962)

#### **Johnstown**

Cambria County Library System Glosser Memorial Library Building (1965)

#### Lancaster

Bucknell University Ellen Clarke Bertrand Library Franklin and Marshall College Shadek-Fackenthal Library (1895)

#### Lewisburg

Bucknell University Ellen Clarke Bertrand Library (1963)

#### Mansfleld

Mansfield University Library (1968)

#### Meadville

Allegheny College Lawrence Lee Pelletier Library (1907)

#### Millersville

Millersville University Helen A. Ganser Library (1966)

#### Monessen

Monessen Public Library (1969)

#### **New Castle**

New Castle Public Library (1963)

#### Newton

**Bucks County Community College Library (1968)** 

#### Norristown

Montgomery County-Norristown Public Library (1969)

#### Philadelphia

Drexel University W. W. Hagerty Library (1963) Free Library of Philadelphia (1897) Saint Joseph's University Drexel Library (1974)
Temple University Paley Library (1947)
Temple University Law Library (1979)
U.S. Court of Appeals Third Circuit Library (1973)
University of Pennsylvania Biddle Law Library (1974)
University of Pennsylvania Library (1886)

# **Pittsburgh**

Allegheny County Law Library (1977)
Carnegie Library of Pittsburgh Allegheny Regional Branch (1924)
Carnegie Library of Pittsburgh (1895)
Duquesne University Law Library (1978)
La Roche College John J. Wright Library (1974)
U.S. Bureau of Mines Library (1962)
University of Pittsburgh Hillman Library (1910)
University of Pittsburgh Barco Law Library (1979)

#### **Pottsville**

Pottsville Free Public Library (1967)

#### Reading

Reading Public Library (1901)

#### Scranton

Scranton Public Library (1895)

# **Shippensburg**

Shippensburg University Ezra Lehman Memorial Library (1973)

# Slippery Rock

Bailey Library (1965)

#### **Swarthmore**

Swarthmore College McCabe Library (1923)

#### **University Park**

Pennsylvania State University Libraries Pattee Library (1907)

#### Villanova

Villanova University Law School Pulling Law Library (1964)

# Warren

Warren Library Association Warren Public Library (1885)

#### Waynesburg

Waynesburg College Library (1964)

#### **West Chester**

West Chester University Francis Harvey Green Library (1967)

#### Wilkes-Barre

King's College D. Leonard Corgan Library (1949)

# Williamsport

Lycoming College Library (1970)

#### York

York College of Pennsylvania Schmidt Library (1963)

# Youngwood

Westmoreland County Community College Learning Resources Center (1972)

#### **PUERTO RICO**

# Mayaguez

University of Puerto Rico Mayaguez Campus Library (1928)

#### **Ponce**

Catholic University of Puerto Rico Encarnacion Valdes Library (1966) Catholic University of Puerto Rico School of Law Library (1978)

#### Rlo Pledras

University of Puerto Rico J. M. Lazaro Library (1928)

# **RHODE ISLAND**

# Barrington

Barrington Public Library (1986)

#### Kingston

University of Rhode Island Library (1907)

# Newport

U.S. Naval War College Library (1963)

#### **Providence**

Brown University John D. Rockefeller Jr. Library (unknown) Providence College Phillips Memorial Library (1969) Providence Public Library (1884) Rhode Island College James P. Adams Library (1965) Rhode Island State Law Library (1979) Rhode Island State Library (1895)

# Warwick

Warwick Public Library (1966)

#### Westerly

Westerly Public Library (1909)

#### Woonsocket

Woonsocket Harris Public Library (1977)

#### **SOUTH CAROLINA**

#### Alken

University of South Carolina-Aiken Gregg-Graniteville Library (1989)

#### Charleston

Baptist College at Charleston L. Mendel Rivers Library (1967) The Citadel Military College Daniel Library (1962) College of Charleston Robert Scott Small Library (1869)

#### Clemson

Clemson University Cooper Library (1893)

#### Columbia

Benedict College Library Payton Learning Resources Center (1969) South Carolina State Library (1895) University of South Carolina Coleman Karesh Law Library (1983) University of South Carolina Thomas Cooper Library (1884)

# Conway

University of South Carolina Coastal Carolina College Kimbel Library (1974)

# **Due West**

Erskine College McCain Library (1968)

#### **Florence**

Florence County Library (1967) Francis Marion College James A. Rogers Library (1970)

#### Greenville

Furman University Library (1962) Greenville County Library (1966)

#### Greenwood

Lander College Jackson Library (1967)

#### Lancaster

University of South Carolina-Lancaster Medford Library

# Orangeburg

South Carolina State College Miller F. Whittaker Library (1953)

#### **Rock Hill**

Winthrop College Dacus Library (1896)

# Spartanburg

Spartanburg County Public Library (1967)

# **SOUTH DAKOTA**

#### Aberdeen

Northern State College Beulah Williams Library (1963)

# **Brookings**

South Dakota State University H. M. Briggs Library (1889)

#### Plerre

South Dakota State Library (1973) South Dakota Supreme Court Library (1978)

# Rapid City

Rapid City Public Library (1963)
South Dakota School of Mines and Technology Devereaux Library (1963)

#### Sloux Falls

Augustana College Mikkelsen Library (1969) Sioux Falls Public Library (1903)

#### Spearfish

Black Hills State University Library E. Y. Berry (1942)

#### Vermillion

University of South Dakota I. D. Weeks Library (1889)

#### **TENNESSEE**

#### **Bristol**

King College E. W. King Library (1970)

# Chattanooga

Chattanooga-Hamilton County Bicentennial Library (1908) U.S. Tennessee Valley Authority Technical Library (1976)

# Clarksville

Austin Peay State University Felix G. Woodward Library (1945)

#### Cleveland

Cleveland State Community College Library (1973)

#### Columbia

Columbia State Community College John W. Finney Memorial Library (1973)

#### Cookeville

Tennessee Technological University Library (1969)

#### **Jackson**

Lambuth College Luther L. Gobbel Library (1967)

# Jefferson City

Carson-Newman College Stephens-Burnett Library (1964)

# Johnson City

East Tennessee State University Sherrod Library (1942)

#### Knoxville

Knoxville County Public Library System Lawson McGhee Library (1973)

University of Tennessee at Knoxville John C. Hodges Library (1907) University of Tennessee Law Library (1971)

#### Martin

University of Tennessee at Martin Paul Meek Library (1957)

# Memphis

Memphis-Shelby County Public Library and Information Center (1896) Memphis State University Cecil C. Humphreys School of Law Library (1979)

Memphis State University Libraries (1966)

#### Murfreesboro

Middle Tennessee State University Todd Library (1912)

# Nashville

Fisk University Library (1965)
Public Library of Nashville and Davidson County (1884)
Tennessee State Library and Archives (unknown)
Tennessee State University Brown-Daniel Library (1972)
Vanderbilt University Alyne Queener Massey Law Library (1976)
Vanderbilt University Library (1884)

#### Sewanee

University of the South Jessie Ball duPont Library (1873)

#### **TEXAS**

#### Abllene

Abilene Christian University Margaret and Herman Brown Library (1978) Hardin-Simmons University Rupert and Pauline Richardson Library (1940)

#### Arlington

Arlington Public Library (1970) University of Texas at Arlington Library (1963)

#### Austin

Texas State Law Library (1972)
Texas State Library (unknown) REGIONAL
University of Texas at Austin Perry-Castaneda Library (1884)
University of Texas at Austin Edie and Lew Wasserman Public Affairs
Library (1966)
University of Texas at Austin Tarlton Law Library (1965)

# **Baytown**

Lee College Library (1970)

#### Beaumont

Lamar University Mary and John Gray Library (1957)

#### **Brownwood**

Howard Payne University Walker Memorial Library (1964)

#### Canyon

West Texas State University Cornette Library (1928)

# **College Station**

Texas Agricultural and Mechanical University Sterling G. Evans Library (1907)

#### Commerce

East Texas State University James Gilliam Gee Library (1937)

# Corpus Christi

Corpus Christi State University Library (1976)

# Corsicana

Navarro College Learning Resource Center (1965)

#### **Dallas**

Dallas Baptist University Vance Memorial Library (1967)
Dallas Public Library (1900)
Southern Methodist University Fondren Library (1925)
University of Texas Southwestern Medical Center Library (1975)

#### Denton

North Texas State University Library (1948)

#### Edinburg

University of Texax-Pan American Library (1959)

#### El Paso

El Paso Public Library (1906) University of Texas at El Paso Library (1966)

#### **Fort Worth**

Fort Worth Public Library (1905) Texas Christian University Mary Couts Burnett Library (1916)

# Galveston

Rosenberg Library (1909)

#### Garland

Nicholson Memorial Library System (1990)

#### Houston

Houston Public Library (1884)
North Harris County College (1974)
Rice University Fondren Library (1967)
South Texas College of Law Library (1981)
Texas Southern University Thurgood Marshall School of Law Library (1982)
University of Houston-Clear Lake Alfred R. Neumann Library (1980)
University of Houston M. D. Anderson Library (1957)
University of Houston School of Law Library (1979)

#### Huntsville

Sam Houston State University Newton Gresham Library (1949)

# irving

Irving Public Library System (1974)

# Kingsville

Texas Arts and Industries University Jernigan Library (1944)

#### Laredo

Laredo Junior College Harold R. Yeary Library (1970)

#### Longview

Longview Public Library (1961)

#### Lubbock

Texas Technical University Library (1935) REGIONAL Texas Technical University School of Law Library (1978)

# **Nacogdoches**

Stephen F. Austin State University Steen Library (1965)

# Richardson

University of Texas at Dallas McDermott Library (1972)

#### San Angelo

Angelo State University Port Henderson Library (1964)

#### San Antonio

Palo Alto College Learning Resources Center Saint Mary's University Academic Library (1964) Saint Mary's University Sarita Kenedy East Law Library (1982) San Antonio College Library (1972) San Antonio Public Library (1899) Trinity University Elizabeth Coates Maddux Library (1964) University of Texas at San Antonio Library (1973)

#### San Marcos

Southwest Texas State University Library (1955)

# Seguin

Texas Lutheran College Blumberg Memorial Library (1970)

#### Sherman

Austin College Abell Library (1963)

#### Texarkana

Texarkana College Palmer Memorial Library (1963)

#### Victoria

Victoria College/University of Houston Victoria Library (1973)

# Waco

Baylor University Caston Law Library (1982) Baylor University Moody Memorial Library (1905)

# Wichita Falls

Midwestern State University Moffett Library (1963)

#### UTAH

# **Cedar City**

Southern Utah State College Library (1964)

# **Ephralm**

Snow College Lucy A. Phillips Library (1963)

#### Logan

Utah State University Merrill Library and Learning Resources Center (1907) REGIONAL

#### Ogden

Weber State College Stewart Library (1962)

#### Provo

Brigham Young University Harold B. Lee Library (1908) Brigham Young University Law Library (1972)

#### Salt Lake City

University of Utah Eccles Health Sciences Library (1970)
University of Utah Law Library (1966)
University of Utah Marriott Library (1893)
Utah State Library (unknown)
Utah State Supreme Court Law Library (1975)

# **VERMONT**

# **Burlington**

University of Vermont Bailey/Howe Library (1907)

#### Castleton

Castleton State College Calvin Coolidge Library (1969)

#### Johnson

Johnson State College John Dewey Library (1955)

# Lyndonville

Lyndon State College Samuel Reed Hall Library (1969)

# Middlebury

Middlebury College Egbert Starr Library (1884)

# Montpeller

Vermont Department of Libraries (1845)

#### Northfield

Norwich University Chaplin Library (1908)

#### South Royalton

Vermont Law School Library (1978)

# **VIRGIN ISLANDS**

#### Saint Croix

Florence Williams Public Library (1968)

#### Saint Thomas

University of the Virgin Islands Ralph M. Paiewonsky Library (1973)

#### **VIRGINA**

#### Alexandria

Dept. of the Navy Office of Judge Advocate General Law Library (1963)

#### Arlington

George Mason University School of Law Library (1981)
U.S. Patent & Trademark Office Scientific and Technical Information
Center (1986)

# Blacksburg

Virginia Polytechnic Institute and State University Carol M. Newman Library (1907)

# **Bridgewater**

Bridgewater College Alexander Mack Memorial Library (1902)

#### Charlottesville

University of Virginia Alderman Library (1910) REGIONAL University of Virginia Arthur J. Morris Law Library (1964)

# Chesapeake

Chesapeake Public Library (1970)

#### Danville

Danville Community College Learning Resources Center (1969)

# **Emory**

Emory and Henry College Kelly Library (1884)

#### **Fairfax**

George Mason University Fenwick Library (1960)

# Fredericksburg

Mary Washington College Library (1940)

# Hampden-Sydney

Hampden-Sydney College Eggleston Library (1891)

#### Hampton

Hampton University Huntington Memorial Library (1977)

#### Harrisonburg

James Madison University Carrier Library (1973)

# Lexington

Virginia Military Institute Preston Library (1874) Washington and Lee University University Library (1910) Washington and Lee University Wilbur C. Hall Law Library (1978)

# Martinsville

Patrick Henry Community College Learning Resource Center (1971)

#### Norfolk

Norfolk Public Library (1895) Old Dominion University Library (1963) U.S. Armed Forces Staff College Library (1963)

#### Petersburg

Virginia State University Johnston Memorial Library (1907)

#### Quantico

Federal Bureau of Investigation Academy Library (1970)
Marine Corps Education Center MCCDC James Carson Breckinridge
Library (1967)

#### Reston

Department of the Interior Geological Survey Library (1963)

#### Richmond

U.S. Court of Appeals Fourth Circuit Library (1973)
University of Richmond Boatwright Memorial Library (1900)
University of Richmond Law School Library (1982)
Virginia Commonwealth University Library Services (1971)
Virginia State Law Library (1973)
Virginia State Library & Archives (unknown)

#### Roanoke

Hollins College Fisburn Library (1967)

#### Salem

Roanoke College Library (1886)

# Williamsburg

College of William and Mary Marshall-Wythe Law Library (1978) College of William and Mary Swern Library (1936)

#### Wise

Clinch Valley College John Cook Wyllie Library (1971)

#### WASHINGTON

#### Bellevue

Bellevue Public Library (1990)

# Bellingham

Western Washington University Mable Zoe Wilson Library (1963)

#### Cheney

Eastern Washington University JFK Library (1966)

#### **Des Moines**

Highline Community College Library (1983)

#### Ellensburg

Central Washington University Library (1962)

#### **Everett**

Everett Public Library (1914)

# Olympia

Evergreen State College Daniel J. Evans Library (1972) Washington State Law Library (1979) Washington State Library (unknown) REGIONAL

# **Port Angeles**

North Olympic Library System (1965)

#### **Pullman**

Washington State University Holland Library (unknown)

#### Seattle

Seattle Public Library (1908)
University of Washington Suzzallo Library (1890)
University of Washington Marian Gould Gallagher Law Library (1969)
U.S. Court of Appeals 9th Circuit Library (1981)

# Spokane

Gonzaga University School of Law Library (1979) Spokane Public Library (1910)

#### Tacoma

Tacoma Public Library (1894)
University of Puget Sound Collins Memorial Library (1938)
University of Puget Sound School of Law Library (1978)

#### Vancouver

Fort Vancouver Regional Library (1962)

#### Walla Walla

Whitman College Penrose Memorial Library (1890)

#### **WEST VIRGINIA**

#### **Athens**

Concord College J. Frank Marsh Library (1924)

#### Bluefield

Bluefield State College Hardway Library (1972)

#### Charleston

Kanawha County Public Library (1952) West Virginia Library Commission (1975) West Virginia Supreme Court Law Library (1977)

#### **Elkins**

Davis and Elkins College Library (1913)

# **Fairmont**

Fairmont State College Library (1884)

# Huntington

Marshall University James E. Morrow Library (1925)

#### Institute

West Virginia State College Drain-Jordon Library (1907)

# Montgomery

West Virginia Institute of Technology Vining Library (1985)

# Morgantown

West Virginia University Library (1907) REGIONAL

#### Salem

Salem-Tolkyo University Benedum Library (1921)

# Shepherdstown

Shepherd College Scarborough Library (1971)

#### Weirton

Mary H. Weir Public Library (1963)

# WISCONSIN

# **Appleton**

Lawrence University Seeley G. Mudd Library (1869)

#### Belolt

Beloit College Col. Robert H. Morse Library (1888)

# Eau Claire

University of Wisconsin-Eau Claire William D. McIntyre Library (1951)

#### Fond du Lac

Fond du Lac Public Library (1966)

#### **Green Bay**

University of WisconsIn-Green Bay Library Learning Center (1968)

#### La Crosse

La Crosse Public Library (1883) University of Wisconsin-La Crosse Murphy Library (1965)

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State Historical Society of Wisconsin Library (1870) REGIONAL
University of Wisconsin-Madison Memorial Library (1939)
University of Wisconsin-Madison Law Library (1981)
Wisconsin State Law Library (unknown)

#### Milwaukee

Alvemo College Library/Media Center (1971)
Marquette University Law Library (1987)
Medical College of Wisconsin, Inc. Todd Wehr Library (1980)
Milwaukee County Law and Reference Library (1934)
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Waukesha Public Library (1966)

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University of Wisconsin-Whitewater Library and Learning Resources (1963)

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Natrona County Public Library (1929)

# Chevenne

Wyoming State Law Library (1977)
Wyoming State Library (unknown) REGIONAL

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Campbell County Public Library (1980)

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University of Wyoming, Coe Library (1907) University of Wyoming Law Library (1978)

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