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*NBS Special Publication 305
Supplement 17*

Publications of the National Bureau of Standards 1985 Catalog

PUBLICATIONS



***U.S. Department of Commerce
National Bureau of Standards***



The National Bureau of Standards¹ was established by an act of Congress on March 3, 1901. The Bureau's overall goal is to strengthen and advance the nation's science and technology and facilitate their effective application for public benefit. To this end, the Bureau conducts research and provides: (1) a basis for the nation's physical measurement system, (2) scientific and technological services for industry and government, (3) a technical basis for equity in trade, and (4) technical services to promote public safety. The Bureau's technical work is performed by the National Measurement Laboratory, the National Engineering Laboratory, the Institute for Computer Sciences and Technology, and the Center for Materials Science.

The National Measurement Laboratory

Provides the national system of physical and chemical measurement; coordinates the system with measurement systems of other nations and furnishes essential services leading to accurate and uniform physical and chemical measurement throughout the nation's scientific community, industry, and commerce; provides advisory and research services to other Government agencies; conducts physical and chemical research; develops, produces, and distributes Standard Reference Materials; and provides calibration services. The Laboratory consists of the following centers:

- Basic Standards² Z
- Radiation Research
- Chemical Physics
- Analytical Chemistry

The National Engineering Laboratory

Provides technology and technical services to the public and private sectors to address national needs and to solve national problems; conducts research in engineering and applied science in support of these efforts; builds and maintains competence in the necessary disciplines required to carry out this research and technical service; develops engineering data and measurement capabilities; provides engineering measurement traceability services; develops test methods and proposes engineering standards and code changes; develops and proposes new engineering practices; and develops and improves mechanisms to transfer results of its research to the ultimate user. The Laboratory consists of the following centers:

- Applied Mathematics
- Electronics and Electrical Engineering²
- Manufacturing Engineering
- Building Technology
- Fire Research
- Chemical Engineering²

The Institute for Computer Sciences and Technology

Conducts research and provides scientific and technical services to aid Federal agencies in the selection, acquisition, application, and use of computer technology to improve effectiveness and economy in Government operations in accordance with Public Law 89-306 (40 U.S.C. 759), relevant Executive Orders, and other directives; carries out this mission by managing the Federal Information Processing Standards Program, developing Federal ADP standards guidelines, and managing Federal participation in ADP voluntary standardization activities; provides scientific and technological advisory services and assistance to Federal agencies; and provides the technical foundation for computer-related policies of the Federal Government. The Institute consists of the following centers:

- Programming Science and Technology
- Computer Systems Engineering

The Center for Materials Science

Conducts research and provides measurements, data, standards, reference materials, quantitative understanding and other technical information fundamental to the processing, structure, properties and performance of materials; addresses the scientific basis for new advanced materials technologies; plans research around cross-country scientific themes such as nondestructive evaluation and phase diagram development; oversees Bureau-wide technical programs in nuclear reactor radiation research and nondestructive evaluation; and broadly disseminates generic technical information resulting from its programs. The Center consists of the following Divisions:

- Inorganic Materials
- Fracture and Deformation³
- Polymers
- Metallurgy
- Reactor Radiation

¹Headquarters and Laboratories at Gaithersburg, MD, unless otherwise noted; mailing address Gaithersburg, MD 20899.

²Some divisions within the center are located at Boulder, CO 80303.

³Located at Boulder, CO, with some elements at Gaithersburg, MD.

*NBS Special Publication 305
Supplement 17*

Publications of the National Bureau of Standards 1985 Catalog



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CATALOG STRUCTURE AND USE

Full bibliographic citations including keywords and abstracts for National Bureau of Standards papers published and entered into the National Technical Information Service (NTIS) collection are cited in the "NBS Publications Announcements" section of this catalog. (Also included are NBS papers published prior to 1985 but not reported in previous supplements of this annual catalog.) Entries are arranged by the COSATI (Committee on Scientific and Technical Information) classification system which consists of 22 broad subject categories (see back cover) and 178 subcategories. Within a subcategory, entries are listed alphanumerically by NTIS order number.

Four additional abbreviated indexes are included to allow the user to identify NBS 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.

NBS papers may also be identified by searching the NTIS database either online via the commercially available DIALOG system 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 NBS 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) and purchase orders should be cited by these numbers. GPO will accept payment by check, money order, VISA, Mastercharge, or deposit account. For availability and price, write to the GPO or telephone (202) 783-3258. Should an NBS 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, Mastercharge, or deposit account. NTIS is the sole source of Federal Information Processing Standards (FIPS), NBS Interagency Reports (NBSIRs), and Grant/Contract Reports (GCRs).

Sometimes, 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 NBS 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 NBS publications (see inside back cover for a description of the various NBS 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.

NBS PUBLICATIONS ANNOUNCEMENTS

SAMPLE ENTRY

5. Behavioral and Social Sciences		NTIS Subject Category	
5A. Administration and Management		NTIS Subcategory	
500,049		Abstract Number	
PB86-136629	PC A03/MF A01	NTIS order number	Availability Price Codes
National Bureau of Standards, Gaithersburg, MD. Inst. for Computer Sciences and Technology.		Corporate or performing organization	
Executive Guide to Software Maintenance.		Report Title	
W. M. Osborne. 1985, 35 p.		Personal authors	Report date Page count
NBS/SP-500/130		Report Number	
Contract F-000000		Contract or grant number	
Keywords: *Management, *Management information systems, Maintenance, . . .		Keywords: * Indicates keyword index entry	
The Guide provides answers to sixty-four key questions about software maintenance.		Abstract	

1.

AERONAUTICS

1B. Aeronautics

500,001
PB85-178333 PC A04/MF A01
Notre Dame Univ., IN. Dept. of Aerospace and Mechanical Engineering.
Numerical Simulations of the Effect of Floor and Ceiling Venting on Fire and Smoke Spread in Aircraft Cabins,
B. P. De Souza, K. T. Yang, and J. R. Lloyd. Feb 85, 72p NBS/GCR-84/479
Grant NB81-NADA-2000

Keywords: *Aircraft cabins, *Aircraft fires, Computerized simulation, Flow measurement, Mathematical models, Smoke, Vents, Ceilings(Architecture), Floors, Fire safety, UNSAFE II computer code.

Several projects have studied the effects of fires on the interior environment of an aircraft. Fires both internal and external to the aircraft were considered. The thrust of the work was to obtain the interior flow field. The flow was calculated using two- and three-dimensional field models with experimental verification in a wind tunnel.

500,002
PB85-207082 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Fire Safety Technology Div.
Thermal Response of Aircraft Cabin Ceiling Materials during a Post-Crash, External Fuel-Spill, Fire Scenario.
Final rept.,
L. Y. Cooper. 1985, 11p
See also PB85-145647. Sponsored by Federal Aviation Administration, Washington, DC.
Pub. in Proceedings of AIAA (American Institute of Aeronautics and Astronautics) Aerospace Sciences

Meeting (23rd), Reno, NV., January 14-17, 1985, AIAA-85-0395, 11p 1985.

Keywords: *Aircraft cabins, *Aircraft fires, *Fire resistant materials, Thermal resistance, Flammability, Tests, Temperature, Fire safety, Algorithms, *Ceilings.

An algorithm is developed to predict the thermal response of aircraft ceiling materials during a post-crash fire scenario. The scenario involves an aircraft's emergency exit doorway which opens directly onto the flames of an external, fuel-spill fire which engulf a large portion of the fuselage. Data of near-ceiling temperatures acquired during a series of eight, full-scale, wide-body aircraft cabin, post-crash test simulations provide indirect validation of the algorithm. These tests involved cabins outfitted with only single, mockup seats. Two other full-scale cabin tests involving fire spread through twenty-one seat arrays with different types of seat construction provide the input data required to exercise the algorithm in evaluations of fully outfitted cabins. Relative to the post-crash scenario, a measure of cabin fire safety is proposed, viz., the post-crash time-to-ceiling-ignition. The measure would be used as a surrogate for the post-crash time available for passengers to safely evacuate the cabin.

3.

ASTRONOMY AND ASTROPHYSICS

3A. Astronomy

500,003

PB86-130085 Not available NTIS
National Bureau of Standards (NML), Boulder, CO.
Quantum Physics Div.

Two Periods of TT Arietis.

Final rept.,
J. R. Thorstensen, J. Smak, and F. V. Hessman.
1985, 9p
Grants NSF-AST81-08691, NSF-AST83-16496
Sponsored by National Science Foundation, Washington, DC.
Pub. in Publications of the Astronomical Society of the Pacific 97, p437-445 May 85.

Keywords: *Binary stars, *Variable stars, Spectroscopy, Photometry, Reprints, *TT Arietis Star.

The authors obtained velocities of the cataclysmic variable TT Ari in its high and intermediate photometric states, with the aim of clarifying the spectroscopic period and demonstrating that the spectroscopic and photometric periods are indeed distinct. It was found that no single period fits all the available data well; however, the original Cowley et al. period fits all the high-state data quite well. The authors conclude that the velocities change phase between the high and the intermediate states.

500,004

PB86-130143 Not available NTIS
National Bureau of Standards (NML), Boulder, CO.
Quantum Physics Div.

Structure Parameters of Galactic Globular Clusters.

Final rept.,
R. F. Webbink. 1985, 37p
Grants NSF-AST83-17916, NSF-AST80-18859
Sponsored by National Science Foundation, Washington, DC.
Pub. in Dynamics of Star Clusters, IAU Symposium No. 113, Princeton, NJ., May 1984, p541-577 1985.

Keywords: Galaxies, *Globular clusters.

Observed and derived structure parameters are tabulated for 154 galactic globular clusters, 7 dwarf spheroidal satellites of the Galaxy, and 6 globular clusters in the Fornax dwarf spheroidal. Observational parameters listed include equatorial coordinates, apparent level of the horizontal branch, reddening, subgiant branch color at the horizontal branch level, limiting and core angular radii, integrated magnitudes, and central surface brightnesses. Derived parameters include galactic coordinates, heliocentric and galactocentric distance, metallicity, limiting and core radii, central relaxation time scale, central mass density, central velocity dispersion, and central escape velocity.

500,005

PB86-132685 Not available NTIS
National Bureau of Standards (NML), Boulder, CO.
Quantum Physics Div.

Cepheid Distances from Blue Main-Sequence Companions.

Final rept.,
E. Boehm-Vitense. 1985, 6p
Grant NSG-5398

Sponsored by National Aeronautics and Space Administration, Washington, DC.

Pub. in Astrophysical Jnl. 296, p169-174, 1 Sep 85.

Keywords: Distance, Reprints, *Cepheid variables.

The absolute visual magnitudes of main-sequence Cepheid companions was determined from their effective temperatures. These are obtained by comparing the measured relative energy distributions with model atmosphere energy distributions. Assuming an average Galactic extinction law, it was found that the distance moduli for the Cepheids should be smaller by $\Delta(m(v) - M(v)) = -0.5$ as compared to the Sandage-Tammann relation.

3B. Astrophysics

500,006

PB85-202927 Not available NTIS
National Bureau of Standards (NML), Boulder, CO.
Quantum Physics Div.

Progress Report on the Analysis of Long Exposure SWP High Resolution Spectra of Cool Stars.

Final rept.,
J. L. Linsky, T. R. Ayres, A. Brown, K. Carpenter, and C. Jordan. 1984, 5p
Grant NGL-06-003-057
Pub. in Proceedings of Future of Ultraviolet Astronomy Based on Six Years of IUE Research, Greenbelt, MD., April 3-5, 1984, NASA Conference Publication 2349, p445-449 1984.

Keywords: Ultraviolet spectra, Dwarf stars, Giant stars, *Stellar chromospheres, Barium stars, Supergiant stars, IUE.

During the last few years the authors have obtained very long exposure, high-dispersion SWP spectra of many stars located throughout the cool half of the HR diagram. These 12-21 hour exposures were obtained by combining NASA and Vilspa shifts so as to obtain the longest possible exposures at times of low background. Included are dwarf stars of spectral type GO V-M2 V, G9.5 III-M5 II giants, G2 Ib-M2 lab supergiants, a number of RS CVn-type systems, and Barium stars. Given the importance of this data set and the many questions that it can answer with appropriate data reduction and extensive modeling efforts the authors summarize briefly what has and is being done with these data.

500,007

PB85-203586 Not available NTIS
National Bureau of Standards (NML), Boulder, CO.
Quantum Physics Div.

Atmospheric Properties of RU Lupi Derived from High- and Low-Resolution IUE Spectra.

A. Brown, M. V. Penston, R. Johnstone, C. Jordan, and N. P. M. Kuin. 1984, 4p
Pub. in Proceedings of the Future of Ultraviolet Astronomy Based on Six Years of IUE Research, Goddard Space Flight Center, April 3-5, 1984, NASA Conf. Publ. 2349, p338-341.

Keywords: *Stellar atmospheres, Ultraviolet spectra, Line width, *RU Lupi Star, Stellar winds, IUE.

High- and low-dispersion spectra of the pre-main sequence star, RU Lupi, have been obtained using both the SWP and LWR cameras. Strong p Cygni line profiles are seen in Mg II and Fe II emission lines, indicating that the lines are formed in the stellar wind of RU Lupi. An increase in transition region line widths is seen with increasing temperature, which cannot be due solely to opacity broadening, thus indicating that kinematic broadening mechanisms (e.g. flows and turbulence) are dominant. The transition region density is about 3×10^{10} to the 10th power/cc derived from the Si III lambda 1892/C III lambda 1909 line ratio. The status of the star's atmospheric modeling of RU Lupi is discussed.

500,008

PB85-207140 Not available NTIS
National Bureau of Standards (NML), Boulder, CO.
Quantum Physics Div.

Ultraviolet, Radio and X-ray Observations of Hybrid Stars.

Final rept.,
S. A. Drake, A. Brown, and J. L. Linsky. 1984, 4p

Pub. in Proceedings of Future of Ultraviolet Astronomy Based on Six Years of IUE Research, Goddard Space Flight Center, April 3-5, 1984, NASA (National Aeronautics and Space Administration) Conf. Publ. 2349, p472-475.

Keywords: *Stars, Extraterrestrial radio waves, Ultraviolet spectra, X rays, Stellar winds, IUE.

In order to understand the nature of the circumstellar regions in the so-called hybrid (-chromosphere) stars, the authors have analyzed existing long wavelength IUE data of these stars, obtained new 6 cm radio observations with the VLA, and compiled all available X-ray observations. The authors conclude that the low-velocity absorption components seen in the Mg II h and k lines of hybrids are almost certainly interstellar and that only the high-velocity components are indicative of the stellar wind speeds.

500,009

PB85-208098 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Mathematical Analysis Div.

Monsieur Georges Lemaitre.

Final rept.,
A. Deprit. 1984, 30p
Pub. in the Big Bang and Georges Lemaitre, p363-392 1984.

Keywords: *Cosmology, *Biographies, Cosmic rays, General relativity, Universe, *Lemaitre Georges, Big bang cosmology.

Biography of the Belgian scientist, author of the Theory of the Expanding Universe and of the Big Bang Theory in Astronomy.

500,010

PB85-225712 Not available NTIS
National Bureau of Standards (NML), Boulder, CO.
Quantum Physics Div.

Predicted Long-Slit, High-Resolution Emission-Line Profiles from Interstellar Bow Shocks.

Final rept.,
A. C. Raga, and K. H. Boehm. Jun 85, 24p
Grant NSF-AST83-14551
Pub. in Astrophysical Jnl., Supplement Series 58, p201-224 Jun 85.

Keywords: *Spectral lines, *Emission spectra, Interstellar matter, Shock waves, Stars, Reprints, Bow waves.

The authors have computed the position-dependent emission-line profiles (called 'position-velocity diagrams' by Choe, Bohm, and Solf) for the lines H(beta), (N II) lambda 6583, (S II) lambda 6731, (O I) lambda 6300, and (O III) lambda 5007 which are formed in a (somewhat simplified) model of a radiating interstellar bow shock of high Mach number. Such models have been suggested as an explanation of the emission-line spectra of Herbig-Haro objects in connection with the 'interstellar bullet model.' Some of the restrictive assumptions used in related earlier work have been eliminated. By comparing the authors results to the recent high-resolution long-slit coude spectra of Herbig-Haro objects (obtained by Bohm and Solf), important similarities are found.

500,011

PB85-226058 Not available NTIS
National Bureau of Standards (NML), Boulder, CO.
Quantum Physics Div.

Sobolev Approximation for Line Formation with Continuous Opacity.

Final rept.,
D. G. Hummer, and G. B. Rybicki. 1 Jun 85, 10p
Grant NSF-AST82-18375
Pub. in Astrophysical Jnl. 293, p258-267, 1 Jun 85.

Keywords: *Spectral lines, Reprints, Radiative transfer, Sobolev approximation.

The Sobolev approximation for line-formation problems in atmospheres with high-speed flows is generalized to include the effects of continuum absorption and emission in the region of the line. The result is very simple, being expressed entirely in terms of known functions with the exception of one quantity of order unity, which is tabulated. Comparison with accurate

numerical solutions for simple problems in plane-parallel geometry shows the approximation to be quite accurate in those regions of the atmosphere where the conditions for the validity of the approximation are satisfied. A three-dimensional version of the theory is given that applies to general geometries.

500,012
PB85-229920 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Molecular Spectroscopy Div.
Observations of the SiC₂ Radical Toward IRC + 10216 at 1.27 Centimeters.
Final rept.,
L. E. Snyder, C. Henkel, J. M. Hollis, and F. J. Lovas. 1985, 6p
Sponsored by National Science Foundation, Washington, DC.
Pub. in *Astrophysical Jnl.* 290, pL29-L33, 1 Mar 85.

Keywords: Molecular spectroscopy, Silicon carbides, Centimeter waves, Free radicals, Radio astronomy, Reprints, *Silicon dicarbide, *Carbon stars.

The first centimeter-wave transition of the recently identified SiC₂ radical has been observed in the envelope of the evolved carbon star IRC + 10216. The excellent agreement between their measured astronomical rest frequency and the predicted frequency, and their measured line intensity support the SiC₂ identification. The high-resolution line profile and mapping data are used to estimate the size of the IRC + 10216 SiC₂ envelope and the abundance of SiC₂ relative to H₂.

500,013
PB85-230720 Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
Optical and Radio Study of the Taurus Molecular Cloud Toward HD 29647.
Final rept.,
R. M. Crutcher. Jan 85, 15p
Sponsored by National Science Foundation, Washington, DC.
Pub. in *Astrophysical Jnl.* 288, p604-617, 15 Jan 85.

Keywords: *Interstellar matter, Radio astronomy, Reprints, *Molecular clouds, Taurus Constellation.

The advantages of combined optical and radio wavelength observations are discussed, and the first such comprehensive study of a dark molecular cloud is described. The line of sight to HD 29647, an eighth magnitude B6-7 IV Ng-Mn star which is behind the outer envelope of Taurus Molecular Cloud 1, has been studied.

500,014
PB86-101938 Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
Unexpected Ultraviolet Variability of Herbig-Haro Object 1.
Final rept.,
E. W. Brugel, K. H. Boehm, J. M. Shull, and E. Boehm-Vitense. 1985, 4p
Grant NAG5-193
Pub. in *Astrophysical Jnl.* 292, pL75-L78, 15 May 85.

Keywords: *Interstellar matter, *Nebulae, Ultraviolet spectra, Variability, Reprints, IUE.

Between 1979 and 1983 the line fluxes of the C IV 1550 and C III 1909 emission lines in HH 1 have decreased monotonically by factors of at least 4-6, while no indications of drastic changes in the optical range (and specifically in the (O III)5007 line) have been found. Our result is based on four IUE spectra obtained by three different groups of observers. These relatively rapid changes can be used to estimate the thickness of the shocked layers and preshock density (eta sub 0). These results suggest a clumpy medium, with (eta sub 0) approx. = 1000/cc, leading to 'truncated' shock waves whose column densities are insufficient to develop complete recombination zones.

500,015
PB86-102464 Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
Photospheres of Hot Stars. 1. Wind Blanketed Model Atmospheres.
Final rept.,
D. C. Abbott, and D. G. Hummer. Jul 85, 17p
Grant NSF-AST82-18375
Pub. in *Astrophysical Jnl.* 294, p286-302, 1 Jul 85.

Keywords: *Stellar atmospheres, Photosphere, Reprints, Stellar winds.

Preliminary to an extensive and detailed comparison of improved non-LTE photospheric models with observations of hot stars made with high photometric accuracy, the authors construct non-LTE stellar atmospheres which account for the radiation reflected back onto the photosphere by line and electron scattering from the wind. The effects of this 'wind blanketing' on the spectrum and internal structure of the atmosphere are given for an example with T_{eff} = 42,000 K, and a wide range of wind density, gravity, and model assumptions. Particular attention is given to the problem of determining T_{eff}.

500,016
PB86-112133 Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
Combined Effect of Potential and Nonpotential Magnetic Fields on Equilibrium in Stellar Atmospheres.
Final rept.,
E. B. Gliner. 1 Aug 84, 10p
Pub. in *Astrophysical Jnl.* 283, n1 p363-372, 1 Aug 84.

Keywords: *Stellar atmospheres, Stellar magnetic fields, Solar corona, Reprints.

An equilibrium in a plasma atmosphere around a gravitating body is considered with regard to both a magnetic field of electrical currents in the atmosphere and a magnetic field originating inside the star. The relation between the combined non-force-free magnetic field and the thermodynamic parameters of atmospheric plasma is treated analytically on the basis of an approach which is discussed in detail. Though restricted by the axisymmetrical situation, the approach allows for multipole structure of a stellar magnetic field and arbitrary radial variation of a toroidal atmospheric magnetic field. Among phenomena caused by the combined magnetic field are inverted altitude run of density in the atmosphere, depletions and excesses in plasma density, 'north-south' atmospheric asymmetry, and inhomogeneous temperature distribution. Subsequent applications are discussed, in particular for the explanation of solar corona asymmetry.

500,017
PB86-128188 Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
Frequent Ultraviolet Brightenings Observed in a Solar Active Region with Solar Maximum Mission.
Final rept.,
J. G. Porter, J. Tommre, and K. B. Gebbie. 1984, 8p
Grant NSG-5318
Sponsored by Air Force Geophysics Lab., Hanscom AFB, MA., and National Aeronautics and Space Administration, Washington, DC.
Pub. in *Astrophysical Jnl.* 283, n2 pt1 p879-886, 15 Aug 84.

Keywords: *Solar activity, Solar ultraviolet radiation, Ultraviolet spectra, Solar spectrum, Reprints.

Observations in the ultraviolet of sites of enhanced intensity within an active region on the Sun reveal frequent and rapid brightenings in Si IV and O IV line emission. These transition region lines were observed with 0.08 s sampling in time using the Ultraviolet Spectrometer and Polarimeter (UVSP) instrument on the Solar Maximum Mission (SMM) satellite. The observations suggest that intermittent heating events of modest amplitude are occurring at many sites within an active region. By selecting the brightest site at any given time within an active region and then sampling its behavior in detail within a 120 s interval, the authors found that about two-thirds of the samples showed variations of the Si IV line intensity. The brightenings typically lasted about 40 s to 60 s, though some were as brief as 20 s. Intensity increases of about 20% to 100% were commonly observed.

500,018
PB86-128865 Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Time and Frequency Div.
Microwave and Far-Infrared Spectra of the SiH Radical.
Final rept.,
J. M. Brown, R. F. Curl, and K. M. Evenson. 1985, 4p
Sponsored by National Aeronautics and Space Administration, Washington, DC.

Pub. in *Astrophysical Jnl.* 292, p188-191, 1 May 1985.

Keywords: *Chemical analysis, *Microwave spectroscopy, *Silanes, Far infrared radiation, Reprints, *Laser spectroscopy.

The frequencies, wavelengths, and line strengths for transitions in the SiH molecule at microwave and far-infrared wavelengths have been calculated from an analysis of its laser magnetic resonance spectrum.

500,019
PB86-128873 Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
Observations of Interstellar Hydrogen and Deuterium Toward Alpha Centauri A.
Final rept.,
W. B. Landsman, R. C. Henry, H. W. Moos, and J. L. Linsky. 1984, 7p
Grant NSG-5393
Sponsored by National Aeronautics and Space Administration, Washington, DC.
Pub. in *Astrophysical Jnl.* 285, n2 p801-807, 15 Oct 84.

Keywords: *Interstellar matter, Ultraviolet spectra, Reprints, IUE.

The authors present a composite profile of the Ly(alpha) emission line of alpha Cen A, obtained from 10 individual spectra with the high-resolution spectrograph aboard the International Ultraviolet Explorer (IUE) satellite. There is excellent overall agreement with two previous Copernicus observations. Interstellar deuterium is detected, and a lower limit is set on the deuterium to hydrogen ratio. In addition, the deuterium bulk velocity appears blueshifted by 8 + or - 2 km/s with respect to interstellar hydrogen, suggesting a non-uniform medium along the line of sight.

500,020
PB86-132677 Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
Blue Companions of Cepheids.
Final rept.,
E. Boehm-Vitense, and C. Proffitt. 1985, 10p
Grant NSG-5398
Sponsored by National Aeronautics and Space Administration, Washington, DC.
Pub. in *Astrophysical Jnl.* 296, p175-184, 1 Sep 85.

Keywords: Binary stars, Ultraviolet spectra, Reprints, *Cepheid variables, IUE.

Twenty-one Cepheids, known or suspected to have blue companions, were studied with the International Ultraviolet Explorer satellite. For 13 of them, companions were indeed seen, though they were generally fainter in the UV than expected. For four Population I Cepheids, the suspected companions were not seen. For none of the Population II Cepheids could a companion be detected. The authors discuss the effective temperatures and luminosities of the companions which could be observed and compare the positions of Cepheids and companions in the T(eff) luminosity diagrams with positions expected from stellar evolution calculations.

500,021
PB86-133550 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD.
Polarization Properties and Time Variations of the SiO Maser Emission of R Leo.
Final rept.,
F. O. Clark, T. H. Troland, G. H. Pepper, and D. R. Johnson. 1984, 11p
Pub. in *Astrophysical Jnl.* 276, n2 pt 1 p572-582, 15 Jan 84.

Keywords: *Masers, Variable stars, Reprints, *R Leo Star, *Silicon oxide masers, Stellar envelopes, Polarization.

The authors have measured the polarization properties of the v=1, J=2-1 SiO circumstellar maser emission from R Leo over a period of three and one half years. As in previous reports, they present data concerning Stokes parameter I, and linear polarization.

500,022
PB86-133584 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD.

Field 3—ASTRONOMY AND ASTROPHYSICS

Group 3B—Astrophysics

SiO Flux Measurements of Variable Stars.

Final rept.,
F. O. Clark, T. H. Troland, G. H. Pepper, and D. R. Johnson. 1984, 5p
Pub. in *Astrophysical Jnl.* 283, n1 pt 1 p174-178, 1 Aug 84.

Keywords: *Variable stars, *Masers, Reprints, *Silicon oxide masers, Infrared astronomy, Stellar envelopes.

The authors report measurements of total flux for six circumstellar SiO maser sources. Both polarizations were measured simultaneously for these highly polarized sources. They compare SiO flux curves with infrared minima and maxima. The SiO flux correlates with the infrared flux, although a characteristic phase lag is present. The comparisons of SiO and infrared flux at light minimum are the most straightforward. Interpreted in terms of observed physical motions associated with these stars, the SiO-infrared phase lag of 63 to 129 days can be used to infer a scale size on the order of 10-13 cm. The corresponding light travel time is of the order of 10-17 cm, which is well outside of the SiO line formation region. The observed phase lag is interpreted as strong evidence against direct stellar infrared radiation as an exciting mechanism for the majority of the SiO flux.

500,023
PB86-136827 Not available NTIS
National Bureau of Standards (NML), Boulder, CO.
Quantum Physics Div.
VLA Observations of A and B Stars with Kilogauss Magnetic Fields.

Final rept.,
S. A. Drake, D. C. Abbott, J. H. Bieging, E. Churchwell, and J. L. Linsky. 1985, 6p
Grant NGL-06-003-057
Sponsored by National Aeronautics and Space Administration, Washington, DC.
Pub. in *Proceedings of Radio Stars Workshop*, Boulder, CO., June 1984, p247-252 1985.

Keywords: *Radio sources(Astronomy), Stellar coronas, Stellar magnetic fields, Early stars.

The serendipitous discovery that the star sigma Ori E (B2 Vp (He Strong)) is a 3.5 mJy radio continuum source at 6 cm has stimulated a radio survey of other early-type stars with strong magnetic fields. No Ap stars have been detected of 8 observed, with typical 3 sigma upper limits of 0.5 mJy at 2 cm. Of 6 Bp stars examined, only HR 1890, also a helium-strong star, was detected. The authors discuss possible emission mechanisms for the observed radio emission, and conclude that nonthermal emission seems the most plausible, on the basis of the present data.

500,024
PB86-136835 Not available NTIS
National Bureau of Standards (NML), Boulder, CO.
Quantum Physics Div.
VLA Radio Continuum Survey of Active Late-Type Giants in Binary Systems: Preliminary Results.

Final rept.,
S. A. Drake, T. Simon, and J. L. Linsky. 1985, 6p
Grant NGL-06-003-057
Sponsored by National Aeronautics and Space Administration, Washington, DC.
Pub. in *Proceedings of Radio Stars Workshop*, Boulder, CO., June 1984, p253-258 1985.

Keywords: *Radio sources(Astronomy), *Binary stars, Giant stars, Stellar chromospheres, Late stars, Mass loss.

The authors have made sensitive survey at 6 cm of active G and K giants in binary systems, including the so-called Long-Period RS CVn stars. The systems observed have orbital periods in the range of about 10 to more than 100 days, and are judged to be active on the basis of their pronounced chromospheric and transition region emission lines and (where available) strong X-ray emission compared to single giants of similar spectral type. Results to date show that strong radio continuum emission at centimeter wavelengths is a common but not universal property of this class of stars. The authors discuss possible correlations between radio luminosity and other properties, such as X-ray luminosity, rotational period, and type of companion.

500,025
PB86-139870 Not available NTIS
National Bureau of Standards (NML), Boulder, CO.
Quantum Physics Div.

Mass Loss from Red Giants: Results from Ultraviolet Spectroscopy.

Final rept.,
J. L. Linsky. 1985, 24p
Grant NGL-06-003-057
Sponsored by National Aeronautics and Space Administration, Washington, DC.
Pub. in *Proceedings of Mass Loss from Red Giants*, Los Angeles, California, June 1984, p31-54 1985.

Keywords: *Giant stars, Ultraviolet spectra, *Red giant stars, *Mass loss, Late stars, Stellar winds, X ray sources, Radiative transfer.

New instrumentation in space, primarily the IUE spacecraft, has enabled the application of ultraviolet spectroscopic techniques to the determination of physical properties and reliable mass loss rates for red giant stars. One important result is the determination of where in the H-R diagram are found stars with hot outer atmospheres and with cool winds. So far it appears that single cool stars, except perhaps for the so-called hybrid stars, have either hot outer atmospheres or cool winds but not both.

500,026
PB86-139888 Not available NTIS
National Bureau of Standards (NML), Boulder, CO.
Quantum Physics Div.
Beyond Lyman Alpha: The New Frontier in Ultraviolet Spectroscopy.

Final rept.,
J. L. Linsky. 1985, 9p
Pub. in *Comments on Astrophysics* 10, n6 p247-255 1985.

Keywords: *Ultraviolet spectroscopy, Far ultraviolet radiation, Interstellar matter, Galaxies, Reprints, Stellar chromospheres, Stellar winds.

Major advances in our understanding of planets, stars, the interstellar medium, and galaxies will come from spectroscopy in the ultraviolet at wavelengths below 1200 Å. While existing spacecraft like IUE and Space Telescope, now under construction, are sensitive only at longer wavelengths, the proposed FUSE/Columbus mission will obtain high resolution spectra in the below 1200 Å region even of faint sources. This comment summarizes the scientific program of such a mission.

500,027
PB86-142379 Not available NTIS
National Bureau of Standards (NML), Boulder, CO.
Quantum Physics Div.
North American Workshop on Cataclysmic Variables and Related Systems (8th),

R. F. Webbink. 1985, 10p
Pub. in *Comments Astrophys.* 10, n5 p189-198 1985.

Keywords: *Binary stars, Reprints, *Cataclysmic variables, White dwarf stars, X ray sources.

When the term 'cataclysmic variable' (CV) was coined by R. P. Kraft, he applied it strictly to eruptive variable stars -- the class included supernova, novae, and dwarf novae. From the beginning, it was clear that supernova were fundamentally different phenomena from novae and dwarf novae. The latter two types of objects had been found to have the same underlying physical nature: a low-mass dwarf star, fillings its Roche lobe, and transferring matter through an accretion disk onto a white dwarf star. Supernovae were quickly dropped as members of this class, but in the years since the term cataclysmic variable has been broadened to include other types of objects which, while they may not display well-developed eruptions, and may not all contain accretion disks, nevertheless share the same interacting red dwarf - white dwarf nature.

500,028
PB86-142668 Not available NTIS
National Bureau of Standards (NML), Boulder, CO.
Quantum Physics Div.
AY Ceti: A Flaring, Spotted Star with a Hot Companion.

Final rept.,
T. Simon, F. C. Fekel, and D. M. Gibson. 1985, 9p
Sponsored by National Aeronautics and Space Administration, Washington, DC.
Pub. in *Astrophysical Jnl.* 295, p153-161, 1 Aug 85.

Keywords: *Binary stars, Radio sources(Astronomy), Ultraviolet spectra, Reprints, *AY Ceti stars, Late stars, X ray sources, White dwarf stars, IUE.

AY Ceti is a late-type single-line spectroscopic binary, a bright X ray source, and a spotted star, as evidenced

by its prominent photometric wave. In this paper, the authors report on observations made with the IUE satellite and the VLA radio interferometer. They conclude that the bright lines and soft X ray emission of AY Ceti arise from the cool primary star, rather than from mass transfer and accretion onto the secondary as has recently been proposed for the similar system 56 Peg.

3C. Celestial Mechanics

500,029
PB85-189413 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Mathematical Analysis Div.
Dynamics of Orbiting Dust under Radiation Pressure.

Final rept.,
A. Deprit. 1984, 30p
Pub. in *The Big Bang and Georges Lemaitre*, p151-180 1984.

Keywords: *Dust, *Orbits, Radiation pressure, Hamiltonian functions, Dynamics, Reprints, Initial value problems, Three dimensional.

For a three-dimensional Keplerian system in the presence of a homogeneous field possibly in uniform rotation, action and angle variables are introduced by canonical transformation in the averaged Hamiltonian truncated at the first order. After substitution, the first order averaged system proves to be integrable. More precisely, it is shown how the orbit space decomposes into a pair of spheres in a three-dimensional space, on which the representative curves are the small circles induced by a finite rotation about a fixed axis. From this intuitive geometric picture follow simple formulas for solving the initial value problem.

4.

ATMOSPHERIC SCIENCES

4A. Atmospheric Physics

500,030
PB85-202612 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Anomalous Atmospheric Spectral Features between 300 and 310 NM Interpreted in Light of New Ozone Absorption Coefficient Measurements.

Final rept.,
R. D. McPeters, and A. M. Bass. 1982, 4p
Sponsored by National Aeronautics and Space Administration, Washington, DC.
Pub. in *Geophysical Research Letters* 9, n3 p227-230 Mar 82.

Keywords: *Albedo, *Ozone, Near ultraviolet radiation, Stratosphere, Atmospheric radiation, Reprints, Absorption coefficients, Nimbus 7 satellite.

Continuous scan data from the solar backscattered ultraviolet instrument on Nimbus 7 reveals real structure in the atmospheric albedo between 300 and 310 nm, a region in which spectral anomalies have been reported in ground based observations. The authors find that these spectral anomalies are largely explained as structure at the one to five percent level in the ozone absorption coefficient as measured by Bass and Paur. Previous ozone absorption coefficient measurements were insufficiently accurate to resolve this structure.

500,031
PB85-219913 Not available NTIS
CODATA Task Group on Gas Phase Chemical Kinetics.

Evaluated Kinetic and Photochemical Data for Atmospheric Chemistry: Supplement 2, D. L. Baulch, R. A. Cox, R. F. Hampson, J. A. Kerr, and J. Troe. c1984, 120p
Included in Jnl. of Physical and Chemical Reference Data, v13 n4 p1259-1380 1984. Available from American Chemical Society, 1155 Sixteenth St., N.W., Washington, DC 20036.

Keywords: *Reaction kinetics, *Photochemical reactions, *Vapor phases, *Air pollution, Gases, Dissociation reactions, Temperature, Tables(Data), Halogen compounds, Enthalpy, Nitrogen inorganic compounds, Physical properties, Chemical properties, Pressure, Spectroscopic analysis, Oxygen inorganic compounds, Absorption cross sections, Index terms, *Atmospheric chemistry.

The paper updates and extends previous critical evaluations of the kinetics and photochemistry of gas phase chemical reactions of neutral species involved in atmosphere chemistry. The work has been carried out by the authors under the auspices of the CODATA Task Group on Gas Phase Chemical Kinetics. Data sheets have been prepared for 256 thermal and photochemical reactions, containing summaries of the available experimental data with notes giving details of the experimental procedures. For each reaction, a preferred value of the rate coefficient at 298 K is given together with a temperature dependence where possible. The selection of the preferred value is discussed; and estimates of the accuracies of the rate coefficients and temperature coefficients have been made for each reaction. The data sheets are intended to provide the basic physical chemical data needed as input for calculations which model atmospheric chemistry. A table summarizing the preferred rate data is provided, together with an appendix listing the available data on enthalpies of formation of the reactant and product species.

500,032
PB85-230803 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Contemporary Particulate Carbon.
Final rept.,
L. A. Currie. 1982, 17p
Sponsored by General Motors Research Labs., Warren, MI.
Pub. in Proceedings of the International Symposium on Particulate Carbon, Atmospheric Life Cycle, Warren, Michigan, October 13-14, 1980, p245-260 1982.

Keywords: *Particles, *Air pollution, *Isotopic labeling, *Carbon isotopes, *Chemical analysis, *Radiocarbon dating, Sources, Carbon 13, Fossil fuels, Wood, Urban areas, Rural areas, Biological aerosols, *Natural emissions.

Advances in natural radiocarbon measurement techniques have made it feasible, for the first time, to assess the contribution of biogenic (contemporary) carbonaceous sources to individual chemical fractions in milligram quantities of atmospheric particles. Isotopic measurements for source reconciliation are doubly important when dealing with pure species, such as methane, carbon monoxide or elemental carbon, because they represent the only compositional information obtainable. Elemental carbon is of special interest in this regard because of changing energy patterns associated with both contemporary (wood-burning) and fossil (diesel fuel and unleaded gasoline) carbon. Following a review of the assumptions underlying the use of radiocarbon as a biogenic tracer and the status of minicounter and accelerator techniques for the assay of milligram and microgram samples, a survey will be presented of recent observations on urban and rural carbonaceous particles. Results for these particles, which have been fractionated according to size or volatility, have exhibited the full range from fossil to biogenic source dominance.

500,033
PB86-113982 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Scientific Computing Div.
Solar Cycle Effect on Atmospheric Carbon Dioxide Levels.
Final rept.,
B. L. Kirk, and B. W. Rust. 1983, 8p
Pub. in Weather Clim. Responses. Sol. Var., p129-136 1983.

Keywords: *Atmospheric composition, *Carbon dioxide, *Solar cycle, Solar activity, Sunspots, Ocean temperature, Reprints, Sea surface temperature.

The authors present a causal time-series model for the Mauna Loa atmospheric CO₂ record which supersedes a mathematical model (Rust et al., 1978, 1979) consisting of four effects represented by exponential and sine functions. One effect is a 142-month oscillation which trails the sunspot numbers by exactly a quarter-cycle. This suggests that solar activity affects the rate of change in the atmospheric CO₂ abundance. The new model replaces the mathematical functions with four measured time series representing proposed physical causes and reduces the number of adjustable parameters from 13 to 5 with no significant deterioration in the fit. The authors present evidence that solar activity affects the CO₂ abundance through variations in ocean temperature or circulation.

500,034
PB86-129608 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Autoregressive Representation of Longitudinal, Lateral, and Vertical Turbulence Spectra.
Final rept.,
D. A. Reed, and R. H. Scanlan. 1984, 16p
Pub. in Jnl. of Wind Engineering and Industrial Aerodynamics 17, n2 p199-214 1984.

Keywords: *Wind velocity, Turbulence, Simulation, Spectra, Statistical analysis, Reprints.

A new method for simulation of fluctuating wind velocity time histories based on a combination of time series models and existing expressions for longitudinal, lateral, and vertical turbulence spectra is outlined. Related expressions for calculating the integral scale of turbulence, $(x)_{Lu}$, are presented. Calculated values of $(x)_{Lu}$ using the new method are close to those obtained for various field data.

500,035
PB86-136959 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Gas and Particulate Science Div.
Infrared Band Strengths for Methyl Chloride in the Regions of Atmospheric Interest.
Final rept.,
J. W. Elkins, R. H. Kagann, and R. L. Sams. 1984, 11p
Pub. in Jnl. of Molecular Spectroscopy 105, n2 p480-490 1984.

Keywords: *Chloromethanes, *Infrared spectroscopy, *Molecular vibration, *Atmospheric chemistry, *Air pollution, Greenhouse effect, Band spectro, Reprints, *Methane/chloro, *Fourier transform spectroscopy.

The infrared band strengths of seven vibrational band systems of methyl chloride between 3 and 17 micrometers region were measured at 296 ± 1 K using a Fourier transform infrared spectrometer. These results were obtained at a maximum instrumental resolution of 0.06/cm. The authors measurements should be of interest to atmospheric scientists, since methyl chloride may contribute measurably to the global greenhouse effect of the atmosphere.

500,036
PB86-138120 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Center for Analytical Chemistry.
Application of Tunable Diode-Laser Absorption for Trace Stratospheric Measurements of HCL - Laboratory Results.
Final rept.,
A. Fried, R. Sams, and W. W. Berg. 1984, 14p
Pub. in Applied Optics 23, n11 p1867-1880 1984.

Keywords: *Atmospheric chemistry, *Hydrogen chloride, *Trace elements, *Chemical analysis, Absorption, Stratosphere, Concentration(Composition), Experimental design, Reprints, *Laser spectroscopy, *Air pollution detection.

The authors report the results of a laboratory study for detecting the important atmospheric molecule, HCl, using a tunable diode laser coupled to a multipass White cell. In contrast to many such prototype studies, the calibration in this work was carried out near the concentration range of interest and verified using three independent techniques. Employing pathlengths of 40-m, they have demonstrated a detection sensitivity ($S/N=1$) in the 200-300 parts-per-trillion range at pressures around 9 torr.

4B. Meteorology

500,037
PB86-137916 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Building Technology.
Probability-Models for Annual Extreme Water-Equivalent Ground Snow.
Final rept.,
B. Ellingwood, and R. K. Redfield. 1984, 7p
Pub. in Monthly Weather Review 112, n6 p1153-1159 1984.

Keywords: *Snowmelt, Probability theory, Statistical analysis, Loads(Forces), Roofs, Reprints, *Water equivalent, Northeast Region(United States).

A statistical analysis of annual extreme water-equivalents of ground snow (reported as inches of water) measured at 76 weather stations in the northeast quadrant of the United States through the winter of 1979-1980 is presented. The analysis suggests that probability distributions with longer upper tails than the Type I distribution of extreme values are preferable for describing the annual extremes at a majority of sites. Sampling errors and the selection of water-equivalents for planning and design purposes also are described.

5.

BEHAVIORAL AND SOCIAL SCIENCES

5A. Administration and Management

500,038
FIPS PUB 107 PC E14
National Bureau of Standards, Gaithersburg, MD.
Local Area Networks: Baseband Carrier Sense Multiple Access with Collision Detection Access Method and Physical Layer Specifications and Link Layer Protocol. Category: Software and Hardware Standard. Subcategory: Computer Network Protocols.
Federal information processing standards (Final),
R. Rosenthal. c1984, 263p
Three ring vinyl binder also available, North American Continent price \$6.25; all others write for quote.

Keywords: Computer systems hardware, Links, Standards, Specifications, *Computer networks, *Local area networks, *Federal information processing standards, Office automation, Access methods, Open system interconnections.

FIPS 107 is the first of a family of local area network standards that allow different manufacturer's equipment and devices to interconnect through networks. It specifies a network access technique used in office automation applications. The standard provides the mechanical, electrical, functional and procedural specifications and link protocol required to establish physical connections, to transmit bits and to send data link frames between nodes. (Copyright (c) 1984, The Institute of Electrical and Electronics Engineers, Inc.)

500,039
PB85-179042 PC A06/MF A01
National Bureau of Standards, Gaithersburg, MD. Center for Materials Science.
Journal of Research of the National Bureau of Standards, Volume 89, Number 6, November-December 1984.
1984, 104p
See also PB85-179059 through PB85-179075 and PB85-161271. Also available from Supt. of Docs as

Field 5—BEHAVIORAL AND SOCIAL SCIENCES

Group 5A—Administration and Management

SN703-027-00001-6. Library of Congress catalog card no. 63-37059.

Keywords: *Research projects, Brittleness, Fractography, Ceramics, Nondestructive tests, Toughness, Diffusion, Fatigue(Materials), Crystals, Stress analysis, Thermodynamics, Phase transformation.

Contents:

Indentation fractography:
A measure of brittleness;
Controlled indentation flaws for the construction of toughness and fatigue master maps;
The interactions of composition and stress in crystalline solids.

500,040

PB85-179083 PC A05/MF A01
National Bureau of Standards, Gaithersburg, MD.
Journal of Research of the National Bureau of Standards, Volume 90, Number 1, January-February 1985.

Feb 85, 92p

See also PB85-179091 through PB85-179117 and PB85-161271. Also available from Supt. of Docs as SN703-027-00002-4. Library of Congress catalog card no. 63-37059.

Keywords: *Research projects, Particle size, Density(Mass/volume), Solubility, Fiber optics, Laboratory equipment, Coupled column liquid chromatography, Standard reference materials.

Contents:

Development of a one-micrometer-diameter particle size standard reference material;
Stable low densities and linear relaxation phenomena;
An automated coupled-column liquid chromatography system for measuring aqueous solubilities of hydrophobic solutes;
Fiber optics emphasis on single mode.

500,041

PB85-182772 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Rapid Prototyping of Information Management Systems.

Final rept.,

B. I. Blum, and R. C. Houghton. 1982, 4p
Pub. in Sigsoft Software Eng. Not. 7, n5 p35-38 Dec 82.

Keywords: *Management information systems, *Production management, Prototypes, Systems engineering, Reprints, *Interactive systems, *Software tools, *Computer systems design, User needs.

Rapid prototyping is especially effective when implementing interactive information management systems. With the right tools, the development process for these systems involves the generation of successive prototypes where each successor is closer to the user requirement. The final prototype becomes either the production system or a production subsystem which is integrated into the total system. The tools used to generate successive prototypes are called application generators and program generators. There are several software engineering issues addressed by these tools.

500,042

PB85-187250 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
National Materials Policy: Critical Materials and Opportunities.

Final rept.,

J. B. Wachtman. 1982, 7p
Pub. in American Ceramics Society Bulletin 61, n2 p214-220 1982.

Keywords: Government policies, Reprints, *Critical materials, Advanced materials.

Materials technology is vital and central to high productivity in manufacturing, to efficient energy conversion, to maintaining a high level of health and safety, and to striking a good balance between our standard of living and environmental protection. Recent concern with the possibility of a 'resource war' waged in terms of price escalation or outright cutoff has brought the question of secure supply to the fore. Our advanced technological society requires many very special, high-performance materials. Some of these are almost unique in their ability to perform the required functions. The authors call these critical materials when the function that they perform is very important

and when substitution of other materials significantly lowers performance or increases cost or does both.

500,043

PB85-189322 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Building Technology.
Integration of Construction in the Building Process.

Final rept.,

R. N. Wright. 1984, 5p

Sponsored by Waterloo Univ. (Ontario).

Pub. in Proceedings of Int. Symposium on Organization and Management of Construction (4th), Waterloo, Ontario, Canada, July 22-26, 1984, CIB W-65 1984, 4, p1161-1165.

Keywords: *Construction, *Management, *Buildings, Information systems, Safety, Economics, Organizational structure.

Integration of construction into the whole building process will promote the usefulness, safety and economy of buildings. Advanced information technologies provide technical bases for accomplishing this integration. Participants are encouraged to work with the Working Commission on Organization and Management of Construction of the International Council for Building Research, Studies and Documentation to achieve this integration.

500,044

PB85-196574 (Order as PB85-196541, PC A07/MF A01)
Texas Univ. at Austin.

Automation of the Building Code Compliance,

S. Jaeger, and L. Harelik. Apr 85, 8p

Sponsored by National Bureau of Standards (NEL), Gaithersburg, MD. Center for Building Technology, and National Conference of States on Building Codes and Standards, Inc., Herndon, VA. Prepared in cooperation with Austin Building Inspection Dept., TX. Included in Research and Innovation in the Building Regulatory Process: Proceedings of the NBS/NCSBCS Joint Conference (6th), Technical Seminar on Streamlined Administrative Procedures, Computers in Construction, and Fire Safety Technology held at Denver, Colorado on September 11, 1984, p37-44 Apr 85.

Keywords: *Building codes, Automation, Standards, *Compliance, Computer software.

This is a software development project using microcomputers to check a proposed building project's compliance with the building codes. Plan review and permit procedures in metropolitan building inspection departments are encumbered with a number of problems. Among these are the logistics of processing the increasingly complex construction projects and processing them in a reliable, replicable and consistent manner. This program provides the means toward those ends.

500,045

PB86-102217 PC A04/MF A01
Maryland Univ., College Park. Dept. of Textiles and Consumer Economics.

Implementation of OMB (Office of Management and Budget) Circular A-119: An Independent Appraisal of Federal Participation in the Development and Use of Voluntary Standards.

Final rept.,

S. M. Spivak. May 85, 74p NBS//GCR-85/495

Keywords: *Government policies, *Standards, Government procurement, Evaluation, *Voluntary standards, *Product standards, *Federal agencies, *Regulatory agencies, *OMP Circular A-119, Private organizations.

This study was commissioned by the Office of Product Standards Policy, National Bureau of Standards, as an independent appraisal of the implementation of OMB Circular A-119 (hereinafter referred to as 'A-119' or the 'Circular'). A-119 establishes Federal standards policy for agency participation in the development and use of voluntary standards. This current report is a compendium of numerous interviews and discussions with standards practitioners from both the public and private sectors. It is their collected expertise regarding implementation of A-119 which form the bases for many of the opinions and conclusions summarized herein.

500,046

PB86-111903 Not available NTIS

National Bureau of Standards, Gaithersburg, MD. Office of Product Standards Policy.
Public Sector-Private Sector Standards Interface in the U.S.

Final rept.,

D. R. Mackay. 1982, 5p

Sponsored by Standards Engineering Society, Inc., Minneapolis, MN.

Pub. in Proceedings of Annual Conference on Standards Engineering Society (31st), Ottawa, Ontario (Canada) on September 20-22, 1982, p56-60.

Keywords: *Standards, Policies, *Federal government, Trade Agreements Act.

The paper describes the early history of the involvement of Federal agencies in voluntary standards activities and the recent developments which have modified the respective roles of private sector organizations and public sector agencies. The impacts of the National Policy in Standards, OMB Circular A-119, the U.S. Trade Agreements Act on the private sector-public sector standards interface are discussed.

500,047

PB86-119195 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Operations Research Div.

Budget Estimates for Replacement of Plant and Facility Equipment at the National Bureau of Standards.

Final rept.,

P. T. Chen, and R. E. Chapman. 1981, 17p

Pub. in ASHRAE (American Society of Heating, Refrigeration and Air-Conditioning Engineers) Transactions 87, n1 p1243-1259 1981.

Keywords: *Budget estimates, *Maintenance, *Equipment replacement, Buildings, Cost analysis, Obsolete equipment, Renovating, Reprints, *National Bureau of Standards.

The study develops a framework, based on service life distributions fitted to data from a published survey, for dealing with the 'replacement problem.' Service life distributions are used to develop replacement schedules for approximately 50 major plant and facility equipment items at the National Bureau of Standards (NBS). The costs associated with these replacement schedules are estimated on an annual basis over a ten-year planning horizon using a probabilistic cost model. Estimates from this model are intended for use in budgeting for replacements over the planning horizon. The results of this study indicate that approximately \$11 million (all estimates are in first quarter 1980 dollars) will be needed to meet expected replacements during fiscal years 1982 through 1991 at the NBS Gaithersburg site.

500,048

PB86-128758 PC A03/MF A01
National Bureau of Standards, Gaithersburg, MD. Center for Programming Science and Technology.

Starting and Operating a Microcomputer Support Center,

A. T. Landberg, and S. Winkler. Oct 85, 41p NBS/SP-500/128

Also available from Supt. of Docs as SN003-003-02683-2. Library of Congress catalog card no. 85-600595.

Keywords: *Management information systems, *Microcomputers, Starting, Operations, Personnel, *Managers, Computing, End use, Support services.

The report identifies and discusses the management issues and resources needed to establish a microcomputer support center. For managers contemplating the establishment of such a center, the report provides information on requirements for staffing, space, equipment, software and operating policies. The information presented is derived from reviews and operational experiences of existing installations in the Federal Government and private sector.

500,049

PB86-136629 PC A03/MF A01
National Bureau of Standards, Gaithersburg, MD. Inst. for Computer Sciences and Technology.

Executive Guide to Software Maintenance,

W. M. Osborne. 1985, 35p NBS/SP-500/130

Paper copy available from Supt. of Docs. SN003-003-02685-9.

Keywords: *Management, *Management information systems, Maintenance, Costs, Executives, Guidelines, *Computer software, Software quality control, Computer program reliability, Software configuration management, Software tools, User needs.

The Guide provides answers to sixty-four key questions about software maintenance. It is designed for Federal executives and managers who have a responsibility for the planning and management of software projects. It is also intended for Federal staff members affected by, or involved in, making software changes and who need to be aware of steps that can reduce both the difficulty and cost of software maintenance.

500,050
PB86-137676

(Order as PB86-137627, PC A04/MF A01)
National Bureau of Standards, Gaithersburg, MD.
Metrics and Techniques to Measure Microcomputer Productivity,
W. M. Osborne, and L. Rosenthal. 9 Jul 85, 13p
Included in Jnl. of Research of the National Bureau of Standards, v90 n4 p305-317 Jul-Aug 85.

Keywords: *Office buildings, *Automatic control equipment, *Management information systems, Productivity, Performance evaluation, *Microcomputers, *Information processing.

While it is generally assumed that the use of microcomputers helps to improve productivity in an office environment, quantitative measures in this area are lacking. This paper addresses the measurement of the effect on productivity in an end user, office environment as a result of the introduction of microcomputer-based technology. It is concerned with defining how productivity can be measured in such an environment and with current efforts to measure changes in productivity. It identifies and assesses the various techniques and measures used to describe the magnitude of productivity improvements that result from the use of microcomputers in the workplace, and makes recommendations for ways in which changes in productivity, may be measured.

500,051
PB86-154820 PC A03/MF A01
National Bureau of Standards, Gaithersburg, MD.
Center for Programming Science and Technology.
Guide on Selecting ADP (Automatic Data Processing) Backup Processing Alternatives.
Final rept.,
I. E. Isaac. Nov 85, 43p NBS/SP-500/134.
Also available from Supt. of Docs as SN003-003-02701-4. Library of Congress catalog card no. 85-600618.

Keywords: *Data processing, *Management information systems, *Backup systems, Contingency, Management, Strategy, Alternatives, Computer software.

The publication addresses the issue of selecting ADP backup processing support in advance of events that cause the loss of data processing capability. The document emphasizes the need for managers at all levels of the organization to support the planning, funding, and testing of an alternate processing strategy. It provides a general description of the alternatives, and recommends criteria for selecting the most suitable alternate processing method.

5B. Documentation and Information Technology

500,052
PB85-177640 PC A04/MF A01
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Applied Mathematics.
National Archives and Records Service (NARS) Twenty Year Preservation Plan,
A. Calmes, R. Schofer, and K. R. Eberhardt. 10 Jan 85, 70p NBSIR-85/2999
Sponsored by National Archives and Records Service, Washington, DC.

Keywords: *Maintainability, *Archives, *Documents, *Conservation, Preserving, Evaluation, Inventory control, *National Archives and Records Service, *Preservation plan.

The purpose of this preservation plan is to identify types, extent of programs and resource requirements

to bring the preservation needs of the National Archives and Records Service (NARS) to a current status at the end of twenty-two years. Data for developing the plan was derived from a scientific survey of holdings, data obtained from interviews with NARS' archivists, earlier studies and observation of operations. The recommended plan is divided into nine action categories: (1) environmental control; (2) holdings maintenance of current holdings; (3) holdings maintenance as a part of the accessioning process; (4) interception, assessment and protection at time of use; (5) systematic duplication of impermanent documents; (6) reproduction of frequently used documents; (7) laboratory treatment of intrinsically valuable documents; (8) laboratory conservation of treasures; and (9) preservation of nontextual records. The 22 year cost of the Preservation Plan in 1984 dollars is estimated at \$209.1 million.

500,053
PB85-191948 PC A11/MF A01
National Bureau of Standards, Gaithersburg, MD. Information Resources and Services Div.
NBS (National Bureau of Standards) Library Serial Holdings 1985,
M. L. Kingston. Feb 85, 229p NBSIR-84/2922

Keywords: *Libraries, Proceedings, Periodicals, Documents, Standards, *National Bureau of Standards.

This publication contains holdings information for approximately 4,600 titles held in the NBS Library, representing current and noncurrent journals, periodicals, annuals, memoirs, proceedings, and transactions.

500,054
PB85-221927 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Guide to Locating Sources of Foreign Scientific and Technical Publications.
Final rept.,
J. C. Tucker, and E. Cerutti. 1982, 33p
Pub. in Sciences and Technologies Libraries, n2-4, p79-111 1982.

Keywords: *Information retrieval, Libraries, Bibliographies, Guidelines, Verifying, Sources, Reprints, *Interlibrary loan, *Technical reports, *Foreign documents.

As a result of improved bibliographic reference systems, reduction of library budgets and rising prices of publications, greater demands are made on interlibrary loan staffs to locate material outside the library to satisfy information needs. Traditionally, publications produced outside the United States; particularly by foreign publishers and organizations, have been the most difficult to identify and obtain. The paper investigates different mechanisms for verifying citations to foreign publications and locating sources, including national libraries, online, and commercial sources.

500,055
PB85-226918 CP T02
National Bureau of Standards, Gaithersburg, MD.
Implementation of ANSI (American National Standards Institute) Codes for the Representation of Names of Countries, Dependencies, and Areas of Special Sovereignty for Information Interchange (FIPS PUB 104).
Data file,
J. Newton. 1985, mag tape FIPS PUB-104, NBS/DF/MT-85/002
Data file is available in the EBCDIC and ASCII character sets on 9-track one-half inch tape. Identify recording mode by specifying density and character set. Call NTIS Computer Products if you have questions.

Keywords: *Data file, *Coding, *Countries, Standards, Data, Information processing, Magnetic tapes, *Federal information processing standards, *Geographic areas, Geocoding.

The file contains data from Table 1, updated, of FIPS PUB 104, 'Implementation of ANSI Codes for the Representation of Names of Countries, Dependencies, and Areas of Special Sovereignty for Information Interchange.' The File contains the names, alphabetic two-character codes, and alphabetic three-character codes of each entity listed in FIPS PUB 104. Lack of a code is shown by hyphens (-- or ---). In addition, asterisks for some records indicate whether there is a reserved code for the entity in ISO 3166. A comment field gives additional information about entity, including its name in ISO 3166, if different from that used in FIPS PUB 104. The comments are condensed from the printed version of FIPS PUB 104. Entities are se-

quenced in alphabetic order of their names as they appear in FIPS PUB 104. All names and codes are represented in UPPER CASE. Comments appear in Mixed Case, unless they are alternate names, which appear in UPPER CASE. US BGN is an abbreviation for U.S. Board on Geographic Names.

500,056
PB85-245678 PC A19/MF A01
National Bureau of Standards, Gaithersburg, MD. Information Resources and Services Div.
Publications of the National Bureau of Standards, 1984 Catalog.
Rept. for Jan-Dec 84,
R. J. Morehouse. Jun 85, 441p NBS/SP-305-SUPPL-16
See also PB84-218031. Also available from Supt. of Docs as SN003-003-02667-1.

Keywords: *Catalogs(Publications), Aeronautics, Astronomy, Astrophysics, Atmospheric, Medicine, Sociology, Chemistry, Electronics, Electrical engineering, Materials, Physics, Mechanical engineering, Fuels, Propulsion, Abstracts, US NBS.

The 16th Supplement to Special Publication 305 lists the 1984 papers which reflect the results of National Bureau of Standards programs. Also included are those NBS papers published prior to 1984 but not reported in previous supplements of SP305. In addition to bibliographic data, key words, and abstracts for each publication and/or paper, the catalog provides author, key word, title, and NTIS order/report number indexes.

500,057
PB86-113677 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Office of Standard Reference Data.
Computerized Standard Reference Data.
Final rept.,
B. B. Molino. 1983, 8p
Pub. in Proceedings of International Conference on Computers in Chemical Research and Education (6th), Washington, DC., July 11-16, 1982, Analytical Chemistry Symposia Series, v15 p143-150 1983.

Keywords: *Technological intelligence, Evaluation, Automation, Economic factors, Pricing, *Data management, *Numeric scientific data, *On line systems, References(Standards), Computer applications, Data banks.

In this paper the authors discuss the role of the Office of Standard Reference Data in the critical step of data evaluation in addition to the coordination and stimulation of data activities in the scientific disciplines and technical areas. The authors examine the alterations in these areas of data evaluation and data dissemination which have occurred in the last decade due to advances in computing. The computerization of standard reference data has occurred at all stages of the process, from the automation of the data centers right through the output mechanisms. The advantages of computerized data are discussed, along with a description of the problems encountered. Finally, an overview is given of present products of the Standard Reference Data System, and plans and pricing policies for the future are outlined.

500,058
PB86-113685 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Office of Standard Reference Data.
Activities of the Office of Standard Reference Data in Relation to the Online Distribution of Scientific Numeric Data.
Final rept.,
B. B. Molino, J. R. Rumble, and D. R. Lide. 1982, 9p
Pub. in Proceedings of National Online Meeting, New York, NY., March 31-April 1, 1982, p371-379.

Keywords: *Technological intelligence, Pricing, Evaluation, *Data bases, *Numeric scientific data, *Computer graphics, On line systems, National Bureau of Standards, References(Standards), User needs.

The Office of Standard Reference Data (OSRD) at the National Bureau of Standards administers one of the largest data evaluation networks in the world, the National Standard Reference Data System. Over the last decade, advances in computing have drastically altered both the data evaluation processes and the methods of disseminating these data to the user community. In this paper the authors discuss the implica-

Field 5—BEHAVIORAL AND SOCIAL SCIENCES

Group 5B—Documentation and Information Technology

tions of these changes on the scientific data community, especially with regard to numeric and graphic data. Two specific areas will be dealt with in detail. The first area to be covered deals with the unique features of numeric scientific data, including material descriptions, data modeling, and graphical displays. The key role of scientists in building these data bases is discussed. The second topic is concerned with various economic issues involved with online data systems and numeric scientific data in particular. The cost and price structure for these important data bases will also be discussed.

500,059

PB86-129707 PC A03/MF A01
National Bureau of Standards, Gaithersburg, MD.
Public Information Div.
NBS (National Bureau of Standards) Research Reports, September 1985,
S. Shaffer. Sep 85, 37p NBS/SP-680-4
See also PB85-236354. Library of Congress catalog card no. 85-600575.

Keywords: *Research projects, Ceramics, Fiber optics, Antennas, Optical communication, Preserving, Freezing, Pollution, Magnetic domains, Imaging techniques, Computer software, National Bureau of Standards.

Contents: Research Update; NBS High-Tech Ceramics Program Geared to Needs of Industry; NBS Advanced-Ceramics Expertise, Facilities Available to Industry; Fiber Optics-Lighting the Way to a Communications Revolution; New Technique for Measuring Antenna Performance Pays Off; Seven NBS Inventions Picked as Significant Technological Advances; Assets Frozen as Researchers Put Pollution Problems on Ice; New Instrument Allows Observation of Surface Magnetic Microstructure; Open Systems in Software; New Publications; Conference Calendar.

500,060

PB86-131794 PC A04/MF A01
National Bureau of Standards, Gaithersburg, MD. Inst. for Computer Sciences and Technology.
Issues in the Management of Microcomputer Systems.
Final rept.,
J. Barkley, and L. S. Rosenthal. Sep 85, 56p NBS-SP-500/125
Library of Congress catalog card no. 85-600588.

Keywords: *Microcomputers, *Information systems, Systems management, Data processing, Organizations, *Technology, Strategies.

The document provides general guidance on the management of microcomputer systems. It addresses the need for establishing a management policy and presents background, issues and alternatives which can help an organization in its management and support of microcomputers.

500,061

PB86-138047 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Data Management and Programming Languages Div.
Dictionary Becomes a Tool for System Management.
Final rept.,
D. W. Fife. 1984, 15p
Pub. in *Advances in Data Base Management* 2, p101-115 1984.

Keywords: *Information systems, *Management information systems, *Data processing, Dictionaries, Automation, Systems management, Organizations, Reprints, *Computer software, *Data base management, *Data flow analysis, *Tasks analysis, Technology innovation.

Information system managers have growing interest in an automated dictionary capability to catalog not only data, but also other resources, tasks, information flow, and their relationships within information processing systems. This chapter surveys the technical innovations of the needed software, called an Information Resource Dictionary System, and explains its typical application within an organization.

500,062

PB86-154408 MF E04
National Bureau of Standards, Gaithersburg, MD.
Office of Product Standards Policy.

KWIC Index of U.S. Voluntary Engineering Standards.

Jan 86, 2664p
Supersedes COM 71-50172.
Microfiche copies only (ten sheets of 48X reduction).

Keywords: *Engineering, *Standards,
Indexes(Documentation).

The index contains the permuted titles of more than 28,000 standards, specifications, test methods and recommended practices published by 422 U.S. standards-developing organizations. Each title can be found under all the significant key words which it contains. These key words are arranged alphabetically down the center of each page together with their surrounding context. The date of publication or last revision, the standard number and an acronym designating the standards-issuing organization appear as part of each entry.

500,063

PB86-165354 PC A06/MF A01
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.
FIREDOC Vocabulary List,
N. H. Jason. Sep 85, 112p NBSIR-85/3231

Keywords: *Terminology, *Fire safety, Fires,
Indexes(Documentation), Information retrieval.

The FIREDOC Vocabulary List contains over 4000 entries and reflects the subject matter of published reports, articles and documents comprising the Fire Research Information Services (FRIS). The keywords are geared toward the needs of the users of this collection. The vocabulary was originally used to develop a small fire safety database for NASA/ASRDI (Aerospace Safety Research and Data Institute). FIREDOC is the on-line bibliographic data of this collection.

5C. Economics

500,064

PB85-201762 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Introductory Remarks at the Third International Symposium on Building Economics.
Final rept.,
R. N. Wright. 1984, 2p
Pub. in *Proceedings of Int. Symposium on Building Economics* (3rd), CIB Working Commission W-55, Ottawa, Canada, July 18-20, 1984, p7-8.

Keywords: *Economics, *Buildings, Financial management, Construction management, Decision making, Research, Policies.

Building Economics provides information and techniques needed by policy makers affecting human welfare and the building community and by decision makers in the building process. Participants are encouraged to work with the Working Commission on Building Economics of the International Council for Building Research, Studies and Documentation to advance knowledge and practice in building economics.

500,065

PB85-224707 PC A03/MF A01
National Bureau of Standards, Gaithersburg, MD.
Office of Product Standards Policy.
GATT (General Agreement on Tariffs and Trade) Standards Code Activities of the National Bureau of Standards 1984.
Final rept.,
J. R. Overman. Apr 85, 43p NBSIR-85/3152
See also PB84-218379.

Keywords: *Standards, *International trade, Commerce, Technical assistance, Regulations, Standardization, US NBS, General Agreement on Tariffs and Trade, GATT standards, Certification, Foreign, Domestic.

This report describes the GATT Standards Code activities performed by the Standards Code and Information program, National Bureau of Standards (NBS), for calendar year 1984. NBS responsibilities include operating the U.S. GATT inquiry point for information on standards and certification activities; notifying the GATT Secretariat of proposed U.S. Federal government standards-based rules that may significantly

affect trade; assisting U.S. industry with trade-related standards problems; and responding to inquiries on foreign and U.S. proposed regulations.

500,066

PB86-130044 PC A07/MF A01
National Bureau of Standards, Gaithersburg, MD.
Office of Product Standards Policy.
Proceedings of Conference on International Standards, Gaithersburg, MD., August 1985,
E. A. Vadelund. Aug 85, 128p NBSIR-85/3228

Keywords: *Proceedings, *Meetings, *International trade, *Government procurement, Regulations, *Federal agencies, *Interagency coordination, *International standards, Voluntary standards, Imports.

The Overview of the Conference distills the main themes and points of discussion during the meeting. It identifies the strictures set forth in the OMB Circular A-119 which govern and give guidance to Federal agencies functioning in the international standards arena either as participants or users. Three areas of concern to Federal agencies are identified as suitable topics for the Interagency Committee on Standards Policy to pursue.

500,067

PB86-142098 PC A04/MF A01
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Applied Mathematics.
Impact of Energy Pricing and Discount Rate Policies on Energy Conservation in Federal Buildings.
Final rept.,
S. K. Fuller, and R. T. Ruegg. Nov 85, 61p NBSIR-85/3262
Sponsored by Department of Energy, Washington, DC.

Keywords: Buildings, Fuels, Pricing, *Life-cycle cost, *Energy conservation, Government buildings, Federal Energy Management Program.

The study investigates how energy conservation projects for federal buildings would be affected by a change in energy pricing and discount rate policies. It focuses on the choice between marginal-cost prices versus average market prices and a 10 percent discount rate versus a 7 percent discount rate. Graphical and numerical comparisons of hypothetical cases in selected geographical areas illustrate the expected impact on selection, design and sizing, and priority of energy-saving projects.

500,068

PB86-142148 PC A05/MF A01
National Bureau of Standards, Gaithersburg, MD.
Energy Prices and Discount Factors for Life-Cycle Cost Analysis: Annual Supplement to NBS (National Bureau of Standards) Handbook 135 and NBS Special Publication 709. 1985 Edition,
B. C. Lippiatt, S. F. Weber, and R. T. Ruegg. Nov 85, 97p NBSIR-85/3273
See also PB81-136269. Sponsored by Department of Energy, Washington, DC. Assistant Secretary for Conservation and Renewable Energy.

Keywords: Buildings, Fuels, *Energy conservation, *Life-cycle cost, Government buildings, Federal energy management program.

The report provides the 1985 annual edition of the energy price and discount factor tables used to supplement both the federal life-cycle costing methodology as described in NBS Handbook 135 (HB 135) and private sector life-cycle cost analysis as described as described in NBS Special Publication 709 (SP 709). Tables A (7%), Ba, and C represent revisions of Appendices A, B, and C, respectively, of HB 135. They should be used in life-cycle cost analyses of federal energy conservation projects. Tables A (10%), Bb, and C are to be used in life-cycle cost analyses of federal non-energy conservation projects that require energy price forecasts. The last section of the report, the supplement for private sector life-cycle cost analysis, is identical to Appendix B, Part I of SP 709 and is provided for the convenience of private sector analysts wishing to make use of federal energy price forecasts.

5D. History, Law, and Political Science

500,069
PB85-187565 PC A03/MF A01
 National Bureau of Standards (NEL), Gaithersburg, MD. Law Enforcement Standards Lab.
Guide to Computer-Aided Dispatch Systems.
 Final rept.,
 D. J. Brenner, and M. A. Cadoff. Mar 85, 44p NBSIR-84/2991
 Sponsored by National Inst. of Justice, Washington, DC.

Keywords: Command and control, Procurement, Decision making, Guidelines, Law enforcement, *Communication networks, *Dispatching, Computer system hardware, Computer software.

This guide provides current information on computer-aided dispatch (CAD) systems as they are used by law enforcement and other public safety agencies and is intended to serve as a procurement aid to those persons who are or will be involved with the planning and acquisition of a CAD system. Topics such as the improvements in operations that may result from installation of a CAD system, a description of the system components, various considerations that will require resolution when the decision is made to purchase a CAD system, and provision of sufficient background to enable a knowledgeable purchasing decision to be made are addressed. A general purchase implementation plan is included also.

500,070
PB85-229649 PC A05/MF A01
 National Bureau of Standards, Gaithersburg, MD. Center for Computer Systems Engineering.
Topological Approach to the Matching of Single Fingerprints: Development of Algorithms for Use on Rolled Impressions.
 Final rept.,
 M. K. Sparrow, and P. J. Sparrow. May 85, 80p NBS/SP-500/124
 Also available from Supt. of Docs as SN003-003-02656-5. Library of Congress catalog card no. 85-600541.

Keywords: *Matching, Comparison, Automation, Digital techniques, Topology, Coding, Algorithms, *Fingerprints, *Automated fingerprint processing, Rolled impressions.

The motivation for seeking topological descriptions of single fingerprints is provided by the elasticity of the human skin; successive rolled impressions from the same finger will invariably have suffered a degree of relative distortion (translation, rotation and stretching). Topology based systems should be free from the detrimental effects of plastic distortion. Systems are described for the extraction of simple topological codes from rolled impressions of the pattern types 'loops', 'whorls' and 'arches'. The generated codes take the form of vectors or simple digital arrays. The nature and frequency of changes that may occur in such codes is investigated and fingerprint comparison algorithms, based on these topological codes, are developed. The objective of such algorithms is to draw a score derived from the degree of 'nearness' of the topological codes in such a manner that it intelligently reflects similarity or dissimilarity in the two prints under comparison.

500,071
PB85-230704 Not available NTIS
 National Bureau of Standards, Gaithersburg, MD. Office of the Associate Director for Programs, Budget and Finance.
Infra-technology Support for Indian Industry.
 Final rept.,
 P. L. M. Heydemann. Jun 85, 2p
 Pub. in Indo-American Business Times, Special Issue, p1 Jun 85.

Keywords: *India, *Industries, *Technology transfer, National government.

The author reviews the role of infratechnology services in the drive of the Indian government for industrial expansion and international competitiveness. Industry and agriculture in the U.S. have benefitted greatly from infratechnology support provided by the Federal government. A case is made for setting up similar support organizations in India to facilitate the establishment of new entrepreneurial companies. Such support is particularly necessary for manufacturers of sophisticated, technical products.

500,072
PB86-115672 PC A07/MF A01
 National Bureau of Standards, Gaithersburg, MD.
Uniform Laws and Regulations as Adopted by the National Conference on Weights and Measures (70th), 1985.
 Final rept.,
 C. S. Brickenkamp. Sep 85, 149p NBS/HB-130-1986
 See also PB85-137644. Also available from Supt. of Docs as SN003-003-02676-0.

Keywords: *Law(Jurisprudence), *Regulations, State government, Weight measurement, States(United States), Standardization, Packaging, Units of measurement, Measuring instruments, Commercial laws, Handbooks, Marking, Labels, Sales management, Commodities, Guidelines, Prices, Publicity, Consumer Affairs, National Bureau of Standards, Open dating, *Weights and measures.

The Handbook, 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 this edition includes amendments adopted by the Conference at its Annual Meeting in 1985. The title of the Handbook and the titles of the Laws and Regulations compiled in it were changed at the 1983 Annual Meeting of the NCWM. A completely revised Open Dating Regulation has been added to this year's edition, as has a new index to the Handbook.

500,073
PB86-127552 PC A04/MF A01
 National Bureau of Standards, Gaithersburg, MD. Center for Computer Systems Engineering.
Topological Approach to the Matching of Single Fingerprints: Development of Algorithms for Use on Latent Fingerprints.
 Final rept.,
 M. K. Sparrow, and P. J. Sparrow. Oct 85, 73p NBS/SP-500/126
 Also available from Supt. of Docs as SN003-003-02680-8. Library of Congress catalog card no. 85-600592.

Keywords: *Matching, Comparison, Automation, Digital techniques, Topology, Coding, Algorithms, *Fingerprints, *Automated fingerprint processing, Latent fingerprints.

The paper naturally follows a previous N.B.S. Special Publication (No. 500-124), in which topological coding schemes were devised for automated comparison of rolled impressions. The contents of that paper are a prerequisite for a proper understanding of this one. The development of topological coding schemes is here extended to cover the automated searching of fragmentary latent marks, such as would be found at the scene of a crime. The benefits to be derived from topological descriptions of fingerprints are a direct result of their immunity to change under ordinary plastic distortion. In the case of latent marks such spatial distortions tend to be exaggerated; hence the importance of applying topology-based systems to them. This paper describes a method of coding fingerprint patterns by a variety of 'topological coordinate schemes', with fingerprint comparison being performed on the basis of localized topological information which is extracted from the recorded coordinate sets. Such comparison is shown to offer a substantial improvement in performance over existing (spatial) techniques. Furthermore, a methods for pictorial reconstruction of a complete fingerprint, from its coordinate representation, is demonstrated.

5G. Linguistics

500,074
PB85-229888 Not available NTIS
 National Bureau of Standards, Gaithersburg, MD. Systems Components Div.
Reference Speech Recognition Algorithm for Benchmarking and Speech Data Base Analysis.
 Final rept.,
 J. L. Hieronymus, and W. J. Majurski. 1985, 5p
 Pub. in Proceedings of the Institute of Electrical and Electronic Engineers International Conference on Acoustics, Speech, and Signal Processing, ICASSP 85, Tampa, Florida, March 26-29, 1985, p1573-1576.

Keywords: *Speech recognition, Statistics, Performance, Words(Language), Reprints, Data bases, Data analysis, Benchmarking.

A complete connected word reference algorithm has been developed at NBS. It provides score statistics and confusibility measures as well as word decisions on speech data base on which it is run. The basic algorithm is like the Bridle, Brown, and Chamberlain (1) algorithm with Euclidean distances on mel scale cepstral coefficients. There are options as to the particular spectral features, the type of spectral comparison measures and the training scheme. Score statistics are collected and a measure of confusibility is computed for each word in the vocabulary. The algorithm has been tested on the Texas Instruments Isolated Word Data Base (2). The most confusable words in the data base are no and go. In addition the performance of the reference system has been compared with several generic types of recognizers.

5I. Personnel Selection, Training, and Evaluation

500,075
PB85-202828 Not available NTIS
 National Bureau of Standards, Gaithersburg, MD.
Estimating the Effect of a Large Scale Pretest Posttest Social Program.
 Final rept.,
 C. H. Spiegelman. 1979, 4p
 Pub. in American Statistical Association 1979 Proceedings of the Social Statistics Section, p370-373 1979.

Keywords: *Educational sociology, Tools, Intelligence tests, Statistical analysis, Regression analysis, Errors, Reprints, *Education programs, *Program evaluation, Analysis, G.R.E. scores.

It is well known that nonrandomized education programs are difficult to evaluate (Campbell and Stanley (1968)). Some help in the evaluation may be obtained by using available instrumental variables, such as G.R.E. scores, or I.Q. tests. However, they should be used with great care as errors in these variables can mislead naively performed analysis. The work shown here gives a new procedure for evaluating pretest-posttest social programs. This paper summarizes the most important results and procedures found in Spiegelman (1976, 1977). Examples indicating how and when the new procedure may be useful are found at the end of this paper.

500,076
PB86-129715 PC A03/MF A01
 Hilsenrath (Joseph), Silver Spring, MD.
National Academy of Sciences-National Research Council's Postdoctoral Research Associateship Program: An Account of Its Origin and Early History at the National Bureau of Standards,
 J. Hilsenrath. Sep 85, 40p NBS/GCR-85/500
 Sponsored by National Bureau of Standards, Gaithersburg, MD.

Keywords: History, Tables(Data), Education, Fellowships, *National Bureau of Standards, *Postdoctoral research, National Academy of Sciences.

The report reviews the origins and early history of the National Academy of Sciences-National Research Council's Postdoctoral Research Associateship Program at the National Bureau of Standards. It describes in detail the intra- and interagency discussions and negotiations that led to the program's creation. A number of tables are included with data on such parameters as the associates' disciplines and university affiliations, DOC-NBS awards associates have received, and those still at NBS.

5J. Psychology (Individual and Group Behavior)

500,077
PB85-172526 Not available NTIS
 National Bureau of Standards, Gaithersburg, MD.

Field 5—BEHAVIORAL AND SOCIAL SCIENCES

Group 5J—Psychology (Individual and Group Behavior)

Human Behavior in Fire: What We Know Now.

Final rept.,
B. M. Levin. 1984, 10p
Pub. in SFPE (Society of Fire Protection Engineers)
Technology Report 84-3, 10p 1984.

Keywords: *Human behavior, *Fires, Decision making, Education, Fire protection, Fire alarm systems, Fire safety, Evacuation egress.

While the decisions and actions of people in fire emergencies sometimes may be unpredictable or erratic, it is more common for their decisions and actions to follow consistent behavioral patterns. Fire safety can be upgrading if we design fire safety systems and training programs based on common behavioral patterns. Some common behavioral patterns in fire emergencies are: 1. people will evacuate through a familiar route rather than through the best route; 2. women will tend to warn and assist others while men are more likely to fight the fire; 3. panic is very rare but heroic and altruistic actions are common; 4. many severely disabled people can evacuate themselves in a timely fashion in many buildings if there are no unnecessary barriers; and 5. many people will not respond to mild ambiguous fire cues.

6.

BIOLOGICAL AND MEDICAL SCIENCES

6A. Biochemistry

500,078
PB85-184588 Not available NTIS

National Bureau of Standards, Gaithersburg, MD.
Isolation and Characterization of Radiation Induced Aliphatic Peptide Dimers.

Final rept.,
M. Dizdaroğlu, and M. G. Simic. 1983, 9p
Pub. in International Jnl. of Radiation Biology and Related Studies in Physics, Chemistry and Medicine 44, n3 p231-239 1983.

Keywords: *Peptides, *Separation, *Radiation effects, Gas chromatography, Mass spectroscopy, Reprints, *Hydroxyl radicals, Dimers, High performance liquid chromatography, Succinic acid/diamino-dimethyl.

Alpha-Peptide radicals of L-Ala-L-Ala and tetra-L-Ala, which are formed from OH radical reactions, were shown to give peptide dimers. These peptide dimers were separated and isolated by HPLC. On acid hydrolysis, all of the studied peptide dimers yielded alanine and alpha-diamino methyl succinic acid (Ala-Ala dimer), which was characterized by gas chromatography-mass spectrometry as a TMS derivative. The described procedure is suggested as a suitable method for isolation and characterization of amino acid dimers.

500,079
PB85-205987 Not available NTIS

National Bureau of Standards, Gaithersburg, MD.
Application of Joint Neutron and X-ray Refinement to the Investigation of the Structure of Ribonuclease A at 2.0 Å Resolution.

Final rept.,
A. Wlodawer, and L. Sjolin. 1984, 16p
Pub. in Neutrons in Biology, p349-364 1984.

Keywords: *Biochemistry, *Molecular structure, *Ribonuclease, *Neutron diffraction, *X ray analysis, Proteins, Organic phosphates, Algorithms, Mathematical models, Reprints.

The structure of ribonuclease A has been refined jointly with the neutron and X-ray data extending to 2.0 Å. The results of an earlier X-ray refinement provided the starting model (Wlodawer, A., Bott, R. and Sjolin, L. (1982) Biochemistry 257, 1325-1332). The final R-factor

was 0.159 (X-ray) and 0.183 (neutron) for a model containing all of the atoms expected in the protein, 128 waters, and a phosphate molecule in the active site. The performance of the joint refinement algorithm has been evaluated.

6B. Bioengineering

500,080
PB85-229466 PC A04/MF A01

National Bureau of Standards, Gaithersburg, MD.
Studies of Porous Metal Coated Surgical Implants,
A. C. Fraker, A. W. Ruff, A. C. Van Orden, H. Hahn, and A. J. Bailey. Jun 85, 57p NBSIR-85/3166
Contract FDA-224-79-5023
Prepared in cooperation with ARTECH Corp., Falls Church, VA.

Keywords: *Surgical implants, *Medical equipment, Metals, Biocompatibility, Corrosion, Fatigue, Coatings, *Biomaterials, Cobalt chromium molybdenum alloy, Metal porous coating, Titanium 6 aluminum 4 vanadium alloy.

The material in the report deals with the subject of metal porous coated surgical implants which are used primarily for orthopedic applications. The report is presented in three parts. The first part gives a brief history of the development of various types of metal porous coated implants and discusses the need for improved fixation of orthopedic devices which led to the investigation of porous coatings for bony ingrowth attachment. The second part of the report contains experimental data on the corrosion behavior of sintered spheres of Co-Cr-Mo and analysis of surface films after exposure to saline solution. The third part reports on a corrosion-fatigue study of arc plasma sprayed porous Ti and Ti-6Al-4V coatings. The porous coatings on the materials studied did not adversely affect the corrosion or mechanical properties of the material. Changes in processing, contamination, etc. could have detrimental effects on the chemical and mechanical behavior of the materials.

6E. Clinical Medicine

500,081
PB85-183341 Not available NTIS

National Bureau of Standards, Gaithersburg, MD.
Effects of Ionic Organic Materials on Enamel Demineralization.

Final rept.,
M. S. Tung, and W. E. Brown. 1985, 4p
Sponsored by American Dental Association Health Foundation, Chicago, IL.
Pub. in Caries Research 19, p72-75 1985.

Keywords: *Organic coatings, *Enamels, *Demineralization, *Teeth, Cations, Anions, Dental materials, Reprints.

Effects of charged organic coatings, which changed the permselective properties of enamel, on tooth demineralization were studied. The alternating cationic and anionic coatings render remarkable protection to enamel exposed to an acid buffer.

500,082
PB85-183556 Not available NTIS

National Bureau of Standards, Gaithersburg, MD.
Initiator-Accelerator Systems for Dental Resins.

Final rept.,
G. M. Brauer, and H. Argentar. 1983, 13p
Grant PHS-DE-40015
Pub. in ACS (American Chemical Society) Symposium Series 212, p359-371 1983.

Keywords: *Dental materials, *Acrylic resins, Curing, Plastics, Polymerization, Free radicals, Stability, Sealants, Polymeric films, Reprints, Toluidine/bis(hydroxyethyl), Phenylacetic acid/(dimethylamino), Benzoyl peroxide, Polymerization initiators.

Acrylic resins, because of their excellent esthetic properties, ease of processing and satisfactory biocompatibility, are materials of choice for dental fillings, prosthetic devices and sealants. In practically all applica-

tions, a fluid monomer formulation (sometimes with solid fillers) is hardened by a free-radical-initiated polymerization that is effected by an initiator and/or heat, light or an initiator-accelerator system. Dentures are cured by a heating cycle during which the initiator, usually benzoyl peroxide (BP) is decomposed and releases sufficient radicals to yield a hard denture. Azo compounds such as 2,2-azo-bis-isobutyronitrile may also be used. To provide the cure at ambient or mouth temperature, redox initiator-accelerator systems, generally BP-tertiary aromatic amines, are employed. Many commercial chemical activated restorative resins employ the BP-bis (2-hydroxyethyl)-p-toluidine (DHEPT) system. More reactive amines which yield color stable products, are p-(dimethylamino) phenylacetic acid and its esters. Redox systems such as BP-sulfonic acids, peroxide-thiourea, hydroperoxide-ascorbic acid or trialkylborane-oxygen also cause rapid polymerization of acrylic resins. Their instability on prolonged storage or suspect biocompatibility limits their chemical applications. Cure systems activated by UV or visible light exposure use respectively an aliphatic ether of benzoin or an alpha-diketone such as camphorquinone with a substituted morpholine reducing agent. Light-cure offers a great advantage since this allows the dentist as much working time as he requires.

500,083
PB85-186989 Not available NTIS

National Bureau of Standards, Gaithersburg, MD.
Dental and Medical Materials Group.

Intermediate Restoratives from N-Hexyl Vanillate-EBA-ZnO-Glass Composites.

Final rept.,
G. M. Brauer, and J. W. Stansbury. Nov 84, 6p
Contract PHS-DE-40015
Sponsored by National Inst. of Dental Research, Bethesda, MD.
Pub. in Jnl. of Dental Research 63, n11 p1315-1320 Nov 84.

Keywords: *Dental materials, *Composite materials, Chelates, Additives, Adhesives, Renovating, Glass particle composites, Reprints, *Vanillic acid/(hexylester), Benzoic acid/(ethoxy-ester), Methyl methacrylates, Methacrylic acid/cyclohexyl, Methacrylic acid/dicyclopentadienyloxyethyl.

Vanillate esters such as n-hexyl vanillate (HV) dissolved in a suitable chelating agent - e.g., o-ethoxybenzoic acid (EBA) - react with zinc oxide, aluminum oxide, and hydrogenated rosin powder to yield non-eugenol-containing cements that do not inhibit polymerization and are compatible with acrylic monomers. These cements can be modified by adding methyl methacrylate, or the less-volatile, higher-molecular-weight dicyclopentenylloxyethyl, or cyclohexyl methacrylate to the HV-EBA liquid, and silanized glass to the powder. The cement composites adhere strongly to composites, non-precious metals, or porcelains. Rupture of the bond occurs cohesively within the cement. Because of their high strength, low solubility, and excellent adhesion, these cements, subject to their biocompatibility with dental tissues, show great promise as intermediate restorative resins and in the repair of fractured porcelain or porcelain-to-metal crowns and bridges.

500,084
PB85-189181 Not available NTIS

National Bureau of Standards, Gaithersburg, MD. Polymer Science and Standards Div.

Smear Layer: Removal and Bonding Considerations.

Final rept.,
R. L. Bowen, J. D. Eick, D. A. Henderson, and D. W. Anderson. 1984, 5p
Prepared in cooperation with Oral Roberts Univ., Tulsa, OK. Sponsored by American Dental Association Health Foundation, Chicago, IL.
Pub. in Operative Dentistry, Supplement 3, p30-34 1984.

Keywords: *Dentin, *Abrasives, *Surface chemistry, Adhesions, Chemical bonds, Reprints, Transmission electron microscopy.

A study of cut and abraded dentin surfaces using transmission electron microscopy revealed collagen denaturation to a depth of about one micrometer and loosening of microcracking of the calcified intertubular dentinal structure to a depth of about three micrometers below the surface.

500,085

PB85-195931

Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

Measurement of the X-Ray Induced Light Photons Emitted from Radiographic CaWO₄ Intensifying Screens.

Final rept.,

H. Roehrig, B. Lum, S. Nudelman, M. P. Capp, and C. E. Dick. 1979, 8p

Sponsored by Society of Photo-Optical Instrumentation Engineers, Bellingham, WA.

Pub. in Application of Optical Instrumentation in Medicine (7th), Toronto, Canada, March 25-27, 1979, Proceedings of Society of Photo-Optical Instrumentation Engineering 173, p8-15.

Keywords: *Image intensifiers, *Radiology, *Calcium tungstates, *Luminous intensity, X rays, Reprints.

For calcium tungstate intensifying screens employed in film-screen imaging systems, Coltman found that approximately 1000 light photons of average energy 2.7 eV were produced for each 50 keV x-ray absorbed. Of this number, he found that only about 55% are emitted from the output side of a 109 mg/sq cm screen. The authors have developed a method based on counting single photons to determine this number for various thickness of calcium tungstate screens. For calcium tungstate screens with thicknesses of 30, 50, 86, and 123 mg/sq cm, the average numbers of light photons emitted per absorbed x-ray are measured for 8 x-ray energies between 17- and 69-keV. The values for 50 keV are less than the values found by Coltman. Studies of the causes of this discrepancy are in progress.

500,086

PB85-196145

Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

Studies of Calcified Tissues by Raman Microprobe Analysis.

Final rept.,

M. D. Grynpas, W. J. Landis, and E. S. Etz. 1982, 5p

Sponsored by Microbeam Analysis Society, Bethesda, MD. Pub. in Proceedings of Annual Conference of the Microbeam Analysis Society (17th), Washington, DC., August 9-13, 1982, p333-337.

Keywords: *Raman spectroscopy, *Bioassay, *Bones, *Mineralization, *Calcium, Sampling, Chemical analysis, Laboratory animals, *Microprobe analysis.

Bone samples at various stages of mineralization have been investigated with the NBS developed Raman microprobe. This research parallels both chemical and other microanalytical studies aimed at elucidating the physico-chemical and structural changes of the bone matrix as a function of bone maturation. The samples studied consist of embryonic, young (5-week) and fully-matured (1-year) chicken leg bone for which vibrational Raman spectra have been obtained from microscopic bone particles and thin sections of chick leg bone. These spectra provide qualitative (and semi-quantitative) molecular information on the progressive changes in the mineral and organic composition of these tissues heretofore not further exploitation of the micro-Raman technique as a unique tool for the micro-chemical study of biological mineralization.

500,087

PB85-207041

Not available NTIS

National Bureau of Standards, Gaithersburg, MD. Polymers Div.

Enamel Fluoride Profile Construction from Biopsy Data.

Final rept.,

L. C. Chow, G. M. Beaudreau, and W. E. Brown.

1985, 10p

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

Pub. in Caries Research 19, p103-112 1985.

Keywords: *Enamels, *Fluoride, Biopsy, Reprints.

In fitting enamel biopsy data to a curve that describes the F profile in a subset of individuals subjected to a given treatment regimen, an implicit approximation is made that all individuals of a subset have the same F profile. In the present work the authors assume that the F profiles for the individuals can be best described by a single polynomial functional form, and that the coefficients of the polynomial can be calculated for each individual from multilayered biopsy data. The F content at a normalized depth can then be calculated for each

individual and be used to compute the mean F content of the subset.

500,088

PB85-207264

Not available NTIS

National Bureau of Standards, Gaithersburg, MD. Polymers Div.

Enhanced Fluoride Uptake from Mouthrinses.

Final rept.,

Y. C. Hong, L. C. Chow, and W. E. Brown. Feb 85,

3p

Sponsored by American Dental Association Health Foundation, Washington, DC.

Pub. in Jnl. of Dental Research 64, n2 p82-84 1985.

Keywords: *Fluoride, *Preventive dentistry, Reprints, *Mouthrinses.

It has been shown in laboratory and animal studies that tooth enamel becomes considerably more reactive toward low levels of fluoride after receiving pre-treatment which forms dicalcium phosphate dihydrate (DCPD) in the enamel as an intermediate. This in vitro study was undertaken to determine the effect on human enamel fluoride uptake of incorporating DCPD-forming rinses into a conventional fluoride rinsing program.

500,089

PB85-210409

PC A04/MF A01

National Bureau of Standards, Gaithersburg, MD. Polymers Div.

Properties and Interactions of Oral Structures and Restorative Materials. Annual Report for Period October 1, 1983 through September 30, 1984,

J. A. Tesk, J. M. Antonucci, G. M. Brauer, J. E.

McKinney, and R. W. Penn. Mar 85, 71p NBSIR-85/3119

See also PB84-217587. Sponsored by National Inst. of Dental Research, Bethesda, MD.

Keywords: *Dental materials, *Alloys, Composite materials, Wear resistance, Physical properties, Biomaterials.

The report presents the results of work involved with the development of basic generic science and engineering which is expected to be useful in the development or control of dental materials used for restorative or treatment purposes. Some of the developments involve investigations into new dental resin formulations (Part I) which might improve the performance of dental composites. Cements and adhesion to filler particles or tooth structure are also addressed in this part. Part II deals with examination of the basic parameters affecting the wear and durability of materials with particular emphasis on dental composites. The resultant information is used to help guide developments in Part I. Part III is concerned with dental casting alloys, and the strength of veneered dental systems, in particular, porcelain fused-to-metal.

500,090

PB85-221885

Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

Reference Bases for Accurate Measurement.

Final rept.,

H. T. Yolken. 1983, 10p

Sponsored by American Medical Association, Chicago, IL.

Pub. in American Society for Testing Materials SP-800, p13-21 1983.

Keywords: *Accuracy, Measurements, Standards, Communities, Health, Reprints, *Reference bases.

A rationale is presented to provide for an accuracy based measurement and standards system for use by the health community. The reference base presented relies on a consistent and compatible set of base and derived measurement units, reference measurement methods, standard reference materials and artifacts, evaluated reference data, and instrument calibration services. In addition, the system also includes field measurement methods and instruments, written procedural standards, and measurement assurance programs.

500,091

PB85-229847

Not available NTIS

National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.

Energy Dependence of Radiochromic Dosimeter Response to X-rays and Gamma Rays.

Final rept.,

W. L. McLaughlin, A. Miller, R. M. Uribe, S. Kronenberg, and C. R. Siebert. 1985, 29p

Sponsored by International Atomic Energy Agency, Vienna (Austria), and Federal Emergency Management Agency, Washington, DC.

Pub. in Proceedings of the International Symposium on High-Dose Dosimetry, Vienna, Austria, October 8-12, 1984, p397-424 1985.

Keywords: *Dosimetry, X rays, Gamma rays, Tissues(Biology), Films, Energy, *Radiochromic dosimeters.

Liquid, solid and liquid-core 'fibre-optics' radiochromic dosimeters were studied for their spectral sensitivity to ionizing photons in the energy range 10 keV to 100 MeV. By comparison of ratios of mass energy-absorption coefficients and mass collision stopping powers of water and biological tissues (fat, muscle and bone), approximate errors due to energy dependence for typical 60Co gamma-ray scattered spectra and to rough simulation of tissues by means of certain additives to radiochromic dosimeters could be estimated. Design of approximate tissue-simulating dosimeters is accomplished by comparing experimental and computational results for various radiochromic films, liquid solutions and liquid-core waveguides. Several experimental tests of energy dependence were made using X- and gamma-rays. For water-, fat-, muscle- or bone-simulation over the photon energy range, chlorides, bromides, triethyl phosphate or dimethyl sulphoxide or a combination of these are added in appropriate concentrations.

500,092

PB86-102431

Not available NTIS

National Bureau of Standards, Gaithersburg, MD. Polymers Div.

Acidic Calcium Phosphate Precursors In Formation of Enamel Mineral.

Final rept.,

W. E. Brown, L. C. Chow, C. Siew, and S. Gruninger. 1984, 6p

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

Pub. in Proceedings of the Symposium on Tooth Enamel (4th), Odawara, Japan, May 24-28, 1984, p8-13.

Keywords: *Dental materials, *Calcium phosphates, *Enamels, In vitro analysis, In vivo analysis, Acids, *Chemical reaction mechanisms, Apatite/hydroxy.

It is slightly over a quarter of a century since octacalcium phosphate (OCP), $\text{Ca}_8\text{H}_2(\text{PO}_4)_6 \cdot 5\text{H}_2\text{O}$, was firmly established to be a member of the family of crystalline calcium phosphates and its relationship to hydroxyapatite (OHAp), $\text{Ca}_5(\text{PO}_4)_3\text{OH}$, was correctly perceived. Yet, despite its involvement in many aspects of calcium phosphate chemistry in vitro, its role in enamel chemistry is frequently ignored. In this paper the authors briefly summarize the reported evidence for the involvement of OCP in enamel formation. They then describe the results of some in vivo experiments which provide close to incontrovertible proof that an acidic precursor is involved in the formation of enamel mineral. The authors then discuss the evidence showing that OCP rather than brushite, $\text{CaHPO}_4 \cdot 2\text{H}_2\text{O}$, or monetite, CaHPO_4 , is the most probable acidic calcium phosphate to be involved in this way.

500,093

PB86-102936

Not available NTIS

National Bureau of Standards, Gaithersburg, MD. Polymers Div.

Improving the Casting Accuracy of Fixed Partial Dentures.

Final rept.,

R. W. Hinman, J. A. Tesk, E. E. Parry, and G. T.

Eden. Apr 85, 6p

Sponsored by National Inst. of Dental Research, Bethesda, MD.

Pub. in Jnl. of Prosthetic Dentistry 53, n4 p466-471 Apr 85.

Keywords: Casting, Alloys, Accuracy, Reprints, *Partial dentures, Denture bases, Prosthodontics.

Recent economic conditions have caused a steady increase in the use of base metal alloys for fixed partial dentures (FPD). Unfortunately, base metal alloys are not as readily soldered as gold-based alloys, which

Field 6—BIOLOGICAL AND MEDICAL SCIENCES

Group 6E—Clinical Medicine

predicates a need for techniques to ensure the accuracy of one-piece multiunit castings of base metal alloys. An investigation of the variables that affect the accuracy of one-piece FPD castings was initiated.

500,094
PB86-122991 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.

Effects of Sequential Calcium Phosphate-Fluoride Rinses on Dental Plaque, Staining, Fluoride Uptake, and Caries in Rats.

Final rept.,
R. J. Shern, L. C. Chow, K. M. Couet, A. Kingman, and W. E. Brown. 1984, 5p
Sponsored by American Dental Association Health Foundation, Chicago, IL.
Pub. in Jnl. of Dental Research 63, n12 p1355-1359 Dec 84.

Keywords: *Fluorides, *Preventive dentistry, *Dentistry, Enamel, Plaque, Reprints, Dental cavities.

Oral rinses which included (1) an acidic calcium phosphate solution containing 0.7 M Ca, 1.9 M PO₄, and saturated with respect to CaHPO₄·2H₂O, and with a pH of 2.0, followed by (2) a 0.52 M fluoride solution, from NaF or SnF₂, were provided to rats once daily for seven days. The investigation consisted of two studies: In the first study, the amounts of dental plaque on the tooth surfaces and fluoride concentrations in the outer enamel were assessed seven days after the last treatment; in the second study, the extent of dental caries was evaluated seven weeks after the last treatment. All rinse sequences containing fluoride provided significant caries protection. The acidic calcium phosphate treatment markedly enhanced the ability of the enamel to acquire fluoride without change of surface morphology. Only the rinse sequences that included stannous fluoride showed significant plaque suppression.

500,095
PB86-124872 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.
Dental Research at the National Bureau of Standards: How It Changed the Practice of Dental Health Service.
Final rept.,
G. C. Paffenbarger, J. A. Tesk, and W. E. Brown. 1985, 7p
Sponsored by American Dental Association Health Foundation, Chicago, IL.
Pub. in Jnl. of the American Dental Association 111, p83-89 Jul 85.

Keywords: History, Standards, Reprints, *Dental research, *National Bureau of Standards, *Amalgams.

A history of dental research at the National Bureau of Standards (NBS) since the inception in 1919 is presented. The initial thrust on dental amalgam by the U.S. Army Dental Corps, the assignment of Dr. Souder to the project and subsequent developments are traced. Difficulties in obtaining support for the early stages of the program following World War I are described. The involvement of the American Dental Association (ADA) in 1928, issuance of the first ADA specification on dental amalgam and the ultimate ramifications on dental (and medical) standards programs throughout the world are described. Patient, dentist and taxpayer benefits from support of the dental research program are shown to exceed the combined budgets of the currently supporting institutions, the NBS, ADA and National Institute of Dental Research.

500,096
PB86-129004 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.
Bonding of Restorative Materials to Dentine: The Present Status in the United States.
Final rept.,
R. L. Bowen. 1985, 5p
Pub. in International Dental Jnl. 35, p155-159 1985.

Keywords: *Adhesion, *Bonding agents, *Dentine, Composites, Enamel, Resins, Reprints.

Adhesion of dental resins and composites to dentine and enamel is a research objective that has been pursued by many investigators for over a quarter of a century. The therapeutic possibilities that would derive from success in these endeavors have been exemplified by the numerous clinical applications that have re-

sulted from bonding various resins to enamel by the acid etch bonding technique. Although etching with aqueous phosphoric acid solutions produces clinically useful bonding to enamel, it does not yield adequate bonding to dentine surfaces, and dentine usually comprises part of the surface to which the restorative material must adhere to successfully repair most dental lesions.

500,097
PB86-130093 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.
Application of an X-ray Image Magnifier to the Microradiography of Dental Specimens.
Final rept.,
S. Takagi, L. C. Chow, W. E. Brown, R. C. Dobbryn, and M. Kuriyama. 1985, 4p
Sponsored by National Inst. of Dental Research, Bethesda, MD.
Pub. in Jnl. of Dental Research 64, n6 p866-869 Jun 85.

Keywords: *Radiography, *Dentistry, X rays, Dentin, Enamel, Teeth, Reprints.

A highly parallel incident x-ray beam combined with x-ray image magnification was used to obtain high-resolution microradiographs of dental specimens. Preliminary results obtained using a rotating anode x-ray generator show that limitations associated with conventional contact microradiography regarding (1) spatial resolution; (2) sample thickness; and (3) sample orientation, relative to the film, were significantly reduced.

500,098
PB86-142478 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.
Role of Octacalcium Phosphate in Subcutaneous Heterotopic Calcification.
Final rept.,
M. S. Tung, and W. E. Brown. 1985, 3p
Sponsored by National Inst. of Dental Research, Bethesda, MD.
Pub. in Calcif. Tissue Int. 37, p329-331 1985.

Keywords: *Tissue(Biology), *Calcification, *Scleroderma, Pathology, Reprints.

Comparison of lattice parameters and morphology of some of the microcrystallites in a subcutaneous heterotopic calcification reported by Daculsi et al. with those of heat-treated octacalcium phosphate (OCP) suggests that OCP is one of the mineral phases in dense globules and one of the precursors for the apatite.

500,099
PB86-142692 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.
Divanillates and Polymerizable Vanillates as Ingredients of Dental Cements.
Final rept.,
J. W. Stansbury, and G. M. Brauer. 1985, 11p
Pub. in Jnl. of Biomedical Materials Research 19, p715-725 1985.

Keywords: *Dental materials, *Polymerization, Chelating agents, Chemical properties, Physical properties, Performance evaluation, Reprints, *Vanillates, *Divanillates, *Metal oxides, Vanillic acid/(hexyl-ester), Benzoic acid/(ethoxy-ester), Vanillic acid/(methacryloylethyl-ester), Divanillic acid/(decamethylene-ester).

Vanillate esters with multifunctional groups that react with metal oxides to give chain-extended molecules have been synthesized. Divanillates were obtained from vanillic acid and the corresponding polymethylenediols. Methacryloylethyl vanillate (MEV) and vanillyl methacrylates were prepared respectively from hydroxyethyl vanillate or vanillyl alcohol and methacryloyl chloride. The properties of cements prepared with liquids incorporating these compounds were determined. These cements, subject to their biocompatibility to oral tissues, could be most useful for a number of dental applications.

500,100
PB86-142817 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Center for Radiation Research.

Experimental Basis for Absorbed-Dose Calculations in Medical Uses of Radionuclides.

Final rept.,
J. S. Robertson, M. J. Berger, J. P. Jones, K. A. Lathrop, and J. W. Poston. 1985, 111p
Pub. in NCRP (National Council on Radiation Protection and Measurements) Report No. 83, 111p 1985.

Keywords: *Dosimetry, Reviews, Estimates, Absorption, Dosage, Reprints, *Radionuclides.

The report reviews the status of the methods used to estimate the radiation absorbed doses to humans from internally deposited radionuclides with the emphasis on medical applications.

6F. Environmental Biology

500,101
PB85-196954 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Miniature Signals and Miniature Counters: Accuracy Assurance via Micro-Processors and Multiparameter Control Techniques.
Final rept.,
L. A. Currie, R. W. Gerlach, G. A. Klouda, R. C. Ruegg, and G. B. Tompkins. 1983, 12p
Pub. in Radiocarbon 25, n2 p553-564 1983.

Keywords: *Radioactive materials, *Air pollution, *Carbon, Gas sampling, Particles, Radiation counters, Quality control, Statistical distributions, Reprints, *Air pollution sampling, *Air pollution detection, Microprocessors, On-line measurement systems.

When radiocarbon signals approach background levels, the validity of assumptions concerning Poisson counting statistics and measurement system stability becomes crucial in interpreting the resultant low-level counting observations. The authors current work is directed toward the on-line monitoring of critical parameters which reflect both the (statistical) nature of the non-Poisson errors and their underlying (physical) causes. Their approach at NBS is based on a multidetector system which sends >60 bits of information/pulse to an on-line microprocessor, followed by the generation of two dimensional spectra and multiparameter correlation and control charts which make possible the identification of specific sources of difficulty within a single unattended counting period.

6H. Food

500,102
PB85-202604 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Radiation Dosimetry in Food Irradiation Technology.
Final rept.,
W. L. McLaughlin, R. M. Uribe, and A. Miller. 1982, 3p
Pub. in Trans. American Nuclear Society 41, p23-25 1982.

Keywords: *Food irradiation, *Dosimetry, Quality assurance, Quality control, Gamma rays, Bremsstrahlung, Electron beams, Reprints, Food preservation.

Routine dosimetry is a valuable means of quality control in the preservation of food by ionizing radiation. The radiations include mainly gamma-ray photons (e.g. (60) Co and (137) Cs gamma rays), bremsstrahlung, and electron beams up to 10 MeV. The dose ranges are about 1 kilorad to several megarad. Because of this relatively wide dose range in food processing and the fairly high dose rates and possible extremes of environmental conditions in a process irradiator, dosimetry can require traceability to standards, i.e. by accurate calibration. Suitable care is also required in the selection of the proper dosimetry system for the purpose at hand. The aim of the present summary is to suggest appropriate methods of dosimetry and routine measurement procedures for achieving quality assurance in radiation processing.

500,103
PB85-229854 Not available NTIS
 National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.
Standardization of High-Dose-Measurement of Electron and Gamma Ray Absorbed Doses and Dose Rates.
 Final rept.,
 W. L. McLaughlin. 1985, 16p
 Pub. in Proceedings of the International Symposium on High-Dose Dosimetry, Vienna, Austria, October 8-12, 1984, p357-371 1985.

Keywords: *Dosimetry, *Heat measurement, Electron beams, Food irradiation, Gamma radiation, Standards.

Intense electron beams and gamma radiation fields are used for sterilizing medical devices, treating municipal wastes, processing industrial goods, controlling parasites and pathogens, and extending the shelf-life of foods. Quality control of such radiation processes depends largely on maintaining measurement quality assurance through sound dosimetry procedures in the research leading to each process, in the commissioning of that process, and in the routine dose monitoring practices. This affords documentation as to whether satisfactory dose uniformity is maintained throughout the product and throughout the process. Therefore, dosimetry at high doses and dose rates must in many radiation processes be standardized carefully, so that 'dosimetry release' of a product is verified. The standardization is initiated through preliminary dosimetry intercomparison studies such as those sponsored recently by the IAEA. This is followed by establishing periodic exercises in traceability to national or international standards of absorbed dose and dose rate.

6L. Medical and Hospital Equipment

500,104
PB85-197499 Not available NTIS
 National Bureau of Standards, Gaithersburg, MD.
Fit of Multiple Unit Fixed Partial Denture Castings.
 Final rept.,
 R. W. Hinman, J. A. Tesk, E. E. Parry, and G. T. Eden. 1981, 1p
 Sponsored by National Inst. of Dental Research, Bethesda, MD.
 Pub. in Jnl. of Dental Research 60, 376p 1981.

Keywords: *Dental materials, Dental prostheses, Casting, Reprints, Prosthodontics.

There exists a general consensus within dentistry that the technique which produces the best fit of fixed partial dentures involves the casting of single units which are subsequently joined by soldering. Base metal alloys unfortunately do not, as a class, lend themselves to soldering as readily as do gold based alloys. The difficulties with soldering these alloys predicate the need for techniques which will maximize the accuracy of one piece multiunit castings. A hardened steel die system has been devised to approximate a maxillary three unit FPD. Pressure formed, annealed wax patterns of nearly invariant dimensions are produced and measured and subsequently compared to the resultant castings.

500,105
PB85-207165 Not available NTIS
 National Bureau of Standards, Gaithersburg, MD.
Post-Curing of Dental Restorative Resin.
 Final rept.,
 W. Wu, and B. M. Fanconi. 1983, 4p
 Sponsored by National Inst. of Dental Research, Bethesda, MD.
 Pub. in Polymer Engineering and Science 23, n13 p704-707 1983.

Keywords: Dental materials, Copolymers, Curing, Reprints, Propenoic acid/methyl-(methylethylidene)bis(phenyleneoxy(hydroxypropanediy))ester.

The post-curing of a BIS-GMA based copolymer system at 37C and 100% RH was monitored using Fourier Transform IR (FT-IR). The dependence of degree of post-curing on the monomer and initiator components was investigated. The further polymerization achieved by elevating the temperature was measured using differential scanning calorimetry (DSC).

500,106
PB85-207249 Not available NTIS
 National Bureau of Standards, Gaithersburg, MD. Polymers Div.
Technique for Characterizing Casting Behavior of Dental Alloys.
 Final rept.,
 R. W. Hinman, J. A. Tesk, R. P. Whitlock, E. E. Parry, and J. S. Durkowski. Feb 85, 5p
 Sponsored by National Inst. of Dental Research, Bethesda, MD. and National Naval Dental Center, Bethesda, MD.
 Pub. in Jnl. of Dental Research 64, n2 p134-138 Feb 85.

Keywords: *Dental materials, *Casting alloys, Behavior, Prosthetic devices, Nickel chromium alloys, Reprints.

A technique for characterizing casting behavior of dental alloys has been developed and tested. The method employs easily reproducible specimen patterns and uses equipment and procedures generally available in dental prosthetic laboratories. A castability value is arrived at by counting complete segments of a cast alloy grid.

500,107
PB86-111945 Not available NTIS
 National Bureau of Standards, Gaithersburg, MD. Polymers Div.
Internal Setting Expansion of a Dental Casting Investment Measured with Strain Gauges.
 Final rept.,
 E. T. Meiser, W. G. de Rijk, J. A. Tesk, R. W. Hinman, and R. A. Hesby. Jun 85, 4p
 Pub. in Jnl. Prosthetic Dentistry 53, n6 p870-873 Jun 85.

Keywords: *Dental materials, *Castings, Cements, Investments, Strain gages, Reprints, Prosthodontics.

Dental casting procedures rely in part on the setting expansion of the casting investment to compensate for the shrinkage of the casting alloy during the solidification and cool down process. The feasibility of monitoring the setting expansion of casting investments by means of strain gauges was investigated, with these strain gauges located near the center of the investment. Two types of configurations were employed: I - strain gauges on a polymeric substrate embedded directly in the investment, II - an augmented retentive form (with plates perpendicular to the substrate) also embedded directly in the investment. Results show that the setting expansion as indicated by the strain gauges is significantly less than the values found by the traditional methods of external measurements and even less than those of the internal measurements previously developed by some of the authors. The addition of a retentive frame (wings) to the gauges reduced the variation in the data obtained and produced expansion values higher than those seen with strain gauges on a flat substrate only. Considering all methods, a very real question arises as to which (if any) of the techniques is valid.

500,108
PB86-123072 Not available NTIS
 National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.
SEM (Scanning Electron Microscopy) Studies of Co-Cr-Mo Surgical Implant Alloy Corrosion Behavior.
 Final rept.,
 A. C. Van Orden, J. L. Chidester, A. C. Fraker, and P. Sung. 1982, 2p
 Pub. in Proceedings of Annual Meeting Electron Microscopy Society of America (40th), Washington, DC., August 9-13, 1982, p520-521.

Keywords: *Surgical implants, Anodic polarization, Corrosion, Cobalt, Chromium, Molybdenum, *Scanning electron microscopy.

The influence of small variations in the composition of Co-Cr-Mo alloys was studied using SEM, energy dispersive x-ray analysis, and electrochemical measurements. SEM and EDX data were correlated with data from in vitro corrosion measurements involving anodic polarization and repassivation measurements. The effects of small variations in alloy composition are evident through SEM and EDX studies of the surface film. The alloy with the highest amount of Fe was shown to have the thickest film. The film was shown to be enriched in Fe, Mo and Si, and depleted in Co and Cr. It

can be concluded from this study, that small variations in alloy composition affect the composition and stability of the passive film formed on the surface of the alloys.

500,109
PB86-124062 Not available NTIS
 National Bureau of Standards, Gaithersburg, MD.
Mechanical Durability of Candidate Elastomers for Blood Pump Applications.
 Final rept.,
 G. B. McKenna, and R. W. Penn. 1982, 6p
 Pub. in Proceedings of World Biomaterials Congress (1st), Baden, Austria, April 12, 1980, Advances in Biomaterials 3, p629-634 1982.

Keywords: Fatigue, Cyclic loads, Failure, Durability, *Blood pumps, *Biomaterials, Circulatory assist devices.

The mechanical durability of an elastomer is a critical factor in its suitability for blood pump applications. In such applications an elastomeric bladder is expected to undergo cyclic stress or strain histories at a frequency of approximately 2 Hz for periods of several years. Test methodologies for characterizing the mechanical durability of such materials do not exist. Based on previous work using an additivity of (or cumulative) damage rule as a framework to describe time dependent failure of both glassy and semicrystalline polymers (1,2), the authors have developed a useful methodology for describing the mechanical durability of elastomers which are candidate materials for blood pump applications. Within this framework, the authors are in the process of characterizing the mechanical durability of a polyolefin rubber, a urethane-silicone copolymer elastomer and a segmented polyurethane elastomer all of which are candidate materials for blood pump applications. The authors have also prepared a standard butyl rubber in out laboratory for use as an interlaboratory control for comparisons with other labs testing the same materials.

500,110
PB86-133378 Not available NTIS
 National Bureau of Standards (NEL), Gaithersburg, MD. Mechanical Production Metrology Div.
NBS (National Bureau of Standards) Hearing Aid Test Procedures and Test Data.
 Final rept.,
 E. D. Burnett, and M. Turica. 1982, 213p
 Sponsored by Veterans Administration, Washington, DC.
 Pub. in Handbook of Hearing Aid Measurement 1982, p8-221.

Keywords: *Medical equipment, Handbooks, Responses, Reprints, *Hearing aids, National Bureau of Standards, Veterans Administration.

The methods used by NBS for testing hearing aids for the Veterans Administration are described. Several possible methods of measuring the acoustic response of hearing aids are discussed, with emphasis on the measurement of the insertion response, which is the method used by NBS. The measurement method for determining the saturation sound pressure level, gain, harmonic distortion, equivalent input noise level, frequency response, telephone coil sensitivity, and directionality are discussed. Samples of the test results are included.

500,111
PB86-140027 Not available NTIS
 National Bureau of Standards, Gaithersburg, MD. Polymers Div.
Mesh Monitor for Casting Characterization.
 Final rept.,
 J. A. Tesk, O. Okuno, R. W. Penn, S. Hirano, and H. R. Kase. 1985, 11p
 Sponsored by National Inst. of Dental Research, Bethesda, MD.
 Pub. in Noble Metals Fabrications and Technology Seminar, p35-45 1985.

Keywords: *Dental materials, *Casting, *Monitors, Alloys.

Numerous new dental casting alloys are appearing on the market. The response of each alloy to casting variables is often incompletely known. It is desirable to have some simple method to monitor and predict the response to changes in casting conditions. A polyester sieve mesh has been found to provide a pattern which serves as an effective monitor.

Field 6—BIOLOGICAL AND MEDICAL SCIENCES

Group 6M—Microbiology:

6M. Microbiology:

500,112
PB86-138583 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Inorganic Materials Div.

Problems Related to Sulfate-Reducing Bacteria in the Petroleum Industry.

Final rept.,
W. P. Iverson, and G. J. Olson. 1984, 23p
Pub. in *Petroleum Microbiology*, p619-641 1984.

Keywords: *Petroleum industry, *Biodeterioration, *Sulfate reducing bacteria, Reviews, Corrosion, Microorganisms, Reprints.

The range of problems caused by sulfate reducing bacteria in the petroleum industry is discussed in the review containing over 100 references. Included in the discussion is a description of newly described species of sulfate reducing bacteria, the occurrence of sulfate reducing bacteria in subsurface environments, mechanisms of bacterial dissimilatory sulfate reduction, and the costly economic problems the petroleum industry faces as a result of the activity of these organisms. Some of the economic problems described are the corrosion of metals, plugging of oilfield reservoirs, and failure of tertiary oil recovery operations. Current and potential future control procedures are described.

6Q. Protective Equipment

500,113
PB85-207306 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Law Enforcement Standards Lab.

Ballistic Resistance of Police Body Armor.

Final rept.
Mar 85, 17p
Sponsored by National Inst. of Justice, Washington, DC.
Pub. in *NIJ (National Inst. of Justice) Standard-0101.02*, 17p Mar 85.

Keywords: *Protective clothing, *Armor, *Ballistic deformation, Penetration, Reprints, Kevlar.

The standard establishes minimum performance requirements and methods of test for the ballistic resistance of police body armor. This standard is a revision of NILECJ-STD-0101.01, dated December 1978. This revision adds performance requirements for level III-A, a requirement to test fabric armor for shots impacting the armor at an incident angle of 30 degrees, and a test method that simulates a multishot assault. In addition, the test round velocity for level IV armor has been changed from 838 plus or minus 15 m (2750 plus or minus 50 ft) per second to 868 plus or minus 15 m (2850 plus or minus 50 ft) per second and the allowable time to test the wet conditioned armor has been increased. The scope of the standard is limited to ballistic resistance only and does not address threats from knives or sharply pointed instruments, a different type of threat.

500,114
PB85-207314 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Law Enforcement Standards Lab.

Riot Helmets and Face Shields.

Final rept.
Oct 84, 21p
Sponsored by National Inst. of Justice, Washington, DC.
Pub. in *NIJ (National Inst. of Justice) Standard-0104.02*, 21p Oct 84.

Keywords: *Protective clothing, *Face shield, *Headgear, Helmet, Reprints.

The standard establishes requirements and methods of test for helmets and face shields to be worn by law enforcement officers during civil disturbances, riots, or other situations that pose a threat of injury from blows to the head. This standard is a revision of and supersedes NIJ Standard-0104.01 dated August 1980. This revision of the standard changes the impact attenuation requirement, deletes the requirement for wet testing of helmets, modifies the requirement and test method for peripheral vision limits, and clarifies test methods and test equipment requirements. The scope

of the standard is limited to riot helmets and face shields. It should be noted that they are not designed to offer protection against gunfire.

6R. Radiobiology

500,115
PATENT-4 489 240 Not available NTIS
Department of Commerce, Washington, DC.

Radiochromic Leuko Dye Real Time Dosimeter, One Way Optical Waveguide.

Patent,
S. Kronenberg, W. L. McLaughlin, and C. R. Siebentritt. Filed 15 Nov 82, patented 18 Dec 84, 4p
PB86-174513, PAT-APPL-6-441 718
Supersedes AD-D009 964.
This Government-owned invention available for U.S. licensing and, possibly, for foreign licensng. Copy of patent available Commissioner of Patent, Washington, DC 20231 \$1.00.

Keywords: *Dosimeters, *Patents, *Dyes, *Optical waveguides, Real time operations, *Leuko dye dosimetry, *Radiochromic waveguide dosimeters, Radiochromic dyes, PAT-CL-250-474.

A radiochromic leuko dye dosimeter includes a plastic tube containing a solution of a radiochromic dye which is sensitive to ionizing radiation, one end of the tube being closed by a reflective surface, the opposite end of the tube being closed by a transparent plug to form a one-way optical waveguide. Light enters the tube through the transparent end thereof and is reflected back and exits through the transparent end. The intensity of the exiting light is measured to determine radiation induced absorption of the leuko dye.

500,116
PB85-222305 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Nuclear Radiation Div.

Calibration Techniques for Neutron Personal Dosimetry.

Final rept.,
C. M. Eisenhauer, J. B. Hunt, and R. B. Schwartz. 1985, 15p
Pub. in *Radiation Protection Dosimetry* 10, n1-4, p43-57 1985.

Keywords: *Dosimeters, *Calibrating, Reprints, *Neutron dosimetry, Dose equivalents.

Techniques for calibrating devices used to estimate neutron dose equivalent are discussed. Procedures are recommended for making such calibrations, and for correcting them for effects such as neutron scattering in air and in the walls of the calibration room. Appropriate neutron source and detector combinations, source anisotropy, and optimum source-detector distances for calibrations are discussed. Corrections for neutron scattering using measurements with shadow cones and fitting procedures for detector response as a function of distance are considered, as are corrections predicted by means of simple analytic expressions.

500,117
PB86-138559 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Nuclear Radiation Div.

Natural Matrix Materials for Low-Level Radioactivity Measurements, Lung and Liver.

Final rept.,
K. G. W. Inn, and J. F. McInroy. 1983, 4p
Pub. in *Proceedings of World Congress of Nuclear Medicine and Biology* (3rd), Paris, France, August 29, 1982, p2912-2915.

Keywords: *Radioactivity, Pathology, Lung, Liver, Reprints.

No abstract available.

6T. Toxicology

500,118
PB85-208080 Not available NTIS

National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.

Combustion Conditions and Exposure Conditions for Combustion Product Toxicity Testing.

Final rept.,
C. Huggett. Oct 84, 20p
Pub. in *Jnl. of Fire Sciences* 2, n5 p328-347 Sep/Oct 84.

Keywords: *Toxicity, *Materials tests, *Fire tests, *Combustion products, Air pollution control, Exposure, Laboratory animals, Dosage, Smoke, Comparison, Hazards, Reprints, *Air pollution effects(Animals), *Indoor air pollution, Air pollution effects(Humans).

A number of procedures have been described in the literature for investigation of the inhalation toxicity of combustion products. There is need for agreement on test methods and test conditions to facilitate communication, allow the exchange of data, and provide a basis for control of hazards due to combustion products in fires. Combustion systems and animal exposure systems which have been employed are classified according to their basic attributes. Simple considerations of limiting stoichiometry in the combustion module can guide the selection of conditions which simulate real fire environments. The dynamics of the exposure system will determine the procedural dose received by the test animal and can be related to real fire exposure. Many past investigations have failed to take adequate account of these fundamental principles.

500,119
PB86-141942 PC A05/MF A01
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.

Exploration of Combustion Limitations and Alternatives to the NBS (National Bureau of Standards) Toxicity Test Method.

B. C. Levin, V. Babrauskas, E. Braun, J. Gurman, and M. Paabo. Nov 85, 87p NBSIR-85/3274
Sponsored by Consumer Product Safety Commission, Bethesda, MD.

Keywords: *Toxicity, *Plastics, *Flammability testing, *Laboratory equipment, *Calorimeters, *Air pollution, Combustion products, Experimental design, Bioassay, Performance evaluation, Assessments, Substitutes, *NBS toxicity test method, *Indoor air pollution, Procedures.

Some limitations and potential limitations of the NBS toxicity screening test method had been identified in earlier work. These limitations have now been explored in greater detail. Also investigated was an alternative combustion system, consisting of a radiant cone heater, identical to the one in the recently developed Cone Calorimeter, an enclosed combustion chamber, and a slightly revised variant of the animal chamber. The new animal chamber was so constructed that, prior to the insertion of the animals, it could be evacuated and then back-filled with a desired sampling of the combustion products. The radiant combustion system showed a different mix of capabilities and limitations compared to the cup furnace combustor in the existing test method. In the present project, the more detailed assessment of the cup furnace operation leads to the recommendation that there is no single, universally preferable combustion environment, but that the cup furnace is adequate for the intended purpose of providing toxicity screening.

500,120
PB86-142676 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.

Preliminary Report of the NFPA Advisory Committee on the Toxicity of the Products of Combustion.

Final rept.,
J. E. Snell. 1984, 6p
Pub. in *Fire Jnl.* 78, n5 p69-71, 73-76 Sep 84.

Keywords: *Combustion products, *Toxicity, *Air pollution, *Smoke, *Fire hazards, *Fire fighting, Hazardous materials, Safety, Public health, Reprints, *Air pollution effects(Humans), *Toxic substances, *Occupational safety and health.

The report summarizes the work of the Advisory Committee on the Toxicity of the Products of Combustion (the NFPA (hereinafter referred to as the TAC). It provides a preliminary report of the TAC that is expected to be available in the Fall. The authors have reached the point of making quantitative estimates of the magnitude of the life safety hazard of smoke toxicity rela-

tive to other life safety threats of fire for specified situations. The authors believe that such estimates can be made now. They will help to: (1) narrow the scope of the smoke toxicity debate to those issues that warrant attention; (2) identify the crucial parameters and related measurement and data needs; and (3) provide practical guidance to those responsible for resolving these issues.

7.

CHEMISTRY

7A. Chemical Engineering

500,121
PB85-178069 PC A07/MF A01
National Bureau of Standards (NEL), Boulder, CO.
Center for Chemical Engineering Technical Activities: Fiscal Year 1984.
Research summary rept. Oct 83-Sep 84,
J. Hord. Feb 85, 130p NBSIR-84/3019
Sponsored by National Research Council, Washington, DC.

Keywords: *Chemical engineering, *Research projects, Fluid mechanics, Thermophysical properties, Measurement.

Technical research activities performed by the Center for Chemical Engineering during the Fiscal Year 1984 are summarized herein. These activities fall within the general categories of process measurement, thermophysical properties data, and chemical engineering science. They embody: development and improvement of measurement principles, measurement standards, and calibration services such as volumetric and mass flow rates, volume, density, and humidity; generation (via accurate measurement and advanced predictive models) of reliable reference data for thermophysical properties of pure fluids, fluid mixtures, and solids of vital interest to industry; and development of improved correlations, models, and measurement techniques for solid-fluid slurry flows, heat and mass transport, mixing, and chemically reacting flows of interest in modern unit operations.

500,122
PB85-182749 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Pore Pressure Buildup in Resonant Column Tests.
Final rept.,
R. M. Chung, F. Y. Yokel, and H. Wechsler. 1984,
15p
Pub. in Jnl. Geotech. Eng. 110, n2 p247-261 Feb 84.

Keywords: *High pressure tests, *Column packings, *Liquefaction, Density(Mass/volume), Columns(Process engineering), Shear strain, Sands, Reprints.

Resonant column tests were performed on fully saturated and dry hollow cylindrical and fully saturated solid cylindrical specimens of Monterey No. 0 sand of 60% relative density subjected to 96 kPa confining pressure. The hollow specimens were tested by torsional excitation and the solid specimens by longitudinal excitation. All specimens, whether previously shaken or not, liquefied at the threshold strain of .012% which was previously identified to be the shear strain below which gross particle displacement is frictionally blocked. The effect of previous shaking on damping ratios and shear moduli was also investigated.

500,123
PB85-205755 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Reference Materials—What They Are and How They Should Be Used.
Final rept.,
J. K. Taylor. 1983, 3p
Pub. in Jnl. of Testing and Evaluation 11, n6 p385-387 1983.

Keywords: *Chemical analysis, *Measurement, Reprints, Standard reference materials, Quality control.

The role of reference materials in monitoring the chemical measurement process is considered. Requirements for reliable reference materials are reviewed. The use of reference material data in estimating the uncertainties of the results of measurements on test samples is discussed.

500,124
PB85-207348 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.
Characterization of Fracture Behavior of Adhesive Joints.
Final rept.,
D. L. Hunston, S. S. Wang, and A. J. Kinloch. 1982, 6p
Pub. in Proceedings of American Chemical Society Meeting (184th), Kansas City, MO., September 12-17, 1982, Organic Coatings and Applied Polymer Science 74, p408-413.

Keywords: *Adhesives, *Composites, Fracture, Epoxy, Stress analysis, Viscoelasticity.

The desire to use adhesives and composites in structural applications has led to a need for a failure prediction capability for the polymers used in such systems. Unfortunately, this task is greatly complicated by the failure load being dependent not only upon the specimen geometry but also on the previous history of loading, temperature, environment, etc. For the tough, rubber-modified polymers that are of most interest for structural applications the effects of previous history can be dramatic. As a result, predictions based on measurements at a single set of conditions can lead to dangerous over or under estimates of the fracture behavior. In an effort to understand this problem the present work has studied the fracture behavior of various polymer formulations using bulk and adhesive joint specimens tested over a wide variety of different thermal and loading histories.

500,125
PB85-230639 Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Chemical Engineering Science Div.
Two-Dimensional Permeate Transport with Facilitated Transport Membranes.
Final rept.,
R. D. Noble. 1984, 11p
Pub. in Separation Science and Technology 19, n8/9 p469-478 1984.

Keywords: *Membranes, *Mathematical models, *Transport properties, *Permeability, *Mass transfer, Experimental design, Comparison, Diffusion, Separation, Physical properties, Reprints, *Hollow fiber membranes.

An analytical model has been developed for steady-state permeate transport with facilitated transport membranes. The model contains no adjustable parameters. The model accounts for both axial permeate transport parallel to the membrane and facilitated permeate transport through the membrane. The model predicts the fraction of permeate separated through the membrane as a function of physical properties and operating conditions. The model was derived for a cylindrical geometry but can be applied to a planar geometry. Also, the model could be used for the simple diffusion case when no facilitation is present. Reasonable agreement with experimental data is presented.

500,126
PB86-105269 PC A10/MF A01
National Bureau of Standards (NEL), Boulder, CO. Chemical Engineering Science Div.
Tables of Industrial Gas Container Contents and Density for Oxygen, Argon, Nitrogen, Helium, and Hydrogen.
B. A. Younglove, and N. A. Olien. Jun 85, 203p
NBS/TN-1079
Also available from Supt. of Docs as SN003-003-02659-0. Sponsored by Compressed Gas Association, Arlington, VA.

Keywords: *Industrial plants, *Density(Mass/volume), *Gas cylinders, *Standards, *Fluids, Tables(Data), Oxygen, Argon, Nitrogen, Helium, Hydrogen, Concentration(Composition), Thermophysical properties, Temperature, Pressure, Standard reference materials.

Custody transfer tables are presented for oxygen, argon, nitrogen, helium, and hydrogen. The tables are based on standard reference data previously compiled by the National Bureau of Standards. Two sets of tables are provided for each fluid. Tables in engineering units cover the range -40 to 130F with pressures from 100 to 10,000 psig. Tables in SI units (density versus pressure and temperature) cover the range 200 to 370 K with pressures from 0.5 to 70 MPa. The tables in engineering units are designed to provide a means of determining the volume of gas at standard conditions contained in a tank given the volume of the tank and the pressure and temperature of the gas within the tank. The publication also includes four examples of use of the tables in calculating tank quantities.

500,127
PB86-110848 PC A06/MF A01
National Bureau of Standards (NEL), Boulder, CO. Center for Chemical Engineering.
Survey of Measurement Needs in the Chemical and Related Industries.
Technical note,
J. Hord. Jul 85, 107p NBS/TN-1087
Also available from Supt. of Docs as SN003-003-02671-9.

Keywords: *Information systems, *Chemical industry, *Measurement, *Surveys, Drug industry, Electronic industry, Measuring instruments, Calibrating, Food industry, Temperature measurement, Flow measurement, Plastics industry, Petroleum industry, Concentration(Composition), Marketing, Tables(Data).

A survey of measurement needs in the chemical and related process industries has been completed, a data base established and reported herein. Sixty-five people responded to the survey, representing the chemical, oil and gas, pharmaceutical, electronic chemicals, energy, instrument manufacturer, food, plastics, and other segments of American industry. The respondents identified: 133 measurement problems of which 106 are defined in detail; 27 measurement needs where no current measurement capability exists (or is known); and three generic measurement areas (flow, composition/concentration, and temperature) in need of improvement. The survey revealed strong demands for improved in-line and in-reactor measurements, in a processing plant environment, to improve process/product quality and to reduce costs. The data base includes instrument (sensor) technical specifications, service conditions, calibration and maintenance requirements, and marketing information.

500,128
PB86-122959 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Chemical Thermodynamics Div.
Equilibria in Aqueous Solutions: Industrial Applications.
Final rept.,
N. C. Scrivner, and B. R. Staples. 1983, 14p
Sponsored by American Inst. of Chemical Engineers, New York.
Pub. in Proceedings of World Congress of Chemical Engineering (2nd), Montreal, Canada, October 4-9, 1981, p349-362 1983.

Keywords: *Industrial plants, *Chemical equilibrium, *Solutions, Thermodynamics, Mathematical models, Gypsum, Solubility, Activity coefficient, pH, Calcium sulfate, Chromium hydroxide, Sodium chloride, Pitzer equations.

The paper discusses industrial applications of thermodynamic theories and empirical developments. The predicted solubility of gypsum as a function of ionic strength (added salts) and as a function of temperature is compared by calculations using 2 models, one using a speciation approach (a commercial computer code) and the other a non-speciation model (the Pitzer equations). The solubility data of Marshall and Slusher for added NaCl has selected and recommended as a test data set for model calculations of gypsum solubility. The effects of common ion, neutral ion, and H(+1) on the solubility of gypsum is illustrated. The effect of pH and ionic strength on the solubility of chromium hydroxide complexes is discussed for another industrial application.

500,129
PB86-128170 Not available NTIS

Field 7—CHEMISTRY

Group 7A—Chemical Engineering

National Bureau of Standards (NEL), Boulder, CO. Chemical Engineering Science Div.

Thermophysical Property Data Generated by the NBS (National Bureau of Standards) Center for Chemical Engineering.

Final rept.,
N. A. Olien, and H. J. Raveche. 1984, 7p
Pub. in AIChE (American Institute of Chemical Engineers) Symposium Series 80, n237 p101-107 1984.

Keywords: *Thermophysical properties, *Chemical engineering, *Research projects, Thermodynamics, Forecasting, Phase transformation, Chemical equilibrium, Fluid mechanics, Reprints, *Reference materials.

The paper describes the current and recent past research of the National Bureau of Standards (NBS) Center for Chemical Engineering (CCE) in the area of thermophysical properties. Included is a description of the approach used which integrates experimental, theoretical, and data evaluation efforts. There is also a summary of the impact of data and its accuracy on the chemical process industry. The major portion of the paper is a detailed description of the property research, especially the publications, of the Center over the past ten years. The results are presented in four tables, listing references of importance in the following areas: Pure Fluid Data, Fluid Mixture Data, Handbooks, Bibliographies, Computer Programs, and Solid Property Data. The paper concludes with a brief description of the future direction to be taken by the NBS-Center for Chemical Engineering in thermophysical properties.

500,130

PB86-130978 PC A07/MF A01

National Bureau of Standards (NEL), Boulder, CO. Chemical Engineering Science Div.

Development of a Performance Test Procedure and Measurement Technique in a Batch Mixing System.

D. M. Ginley. Jul 85, 145p NBSIR-85/3030

Keywords: *Mixing, Batching, Tests, Measurement.

A performance test procedure and measurement technique for a batch mixing system is described using conductivity probes. The design of the automated experimental apparatus is described, and experimental procedures are given. Data collected from the experiments are explained, and a mixtime analysis of the data is performed. Conductivity probe response curves provide a good representation of the system dynamics. Mixtime analysis allows for probe response comparisons to evaluate system geometry and probe location.

500,131

PB86-137957

Not available NTIS

National Bureau of Standards, Gaithersburg, MD. Inorganic Materials Div.

Alkali Vapor Transport in Coal Conversion and Combustion Systems.

Final rept.,
J. W. Hastie, E. R. Plante, and D. W. Bonnell. 1982, 58p

See also PB81-221319. Sponsored by Department of Energy, Morgantown, WV. Morgantown Energy Technology Center.
Pub. in ACS (American Chemical Society) Symposium Series 179, p543-600 1982.

Keywords: *Alkali resistant tests, *Corrosion tests, *Coal, *Combustion chambers, Fuel additives, Transport properties, Mass spectroscopy, Reprints, *Synthetic fuels.

Alkali metal containing vapor species are ubiquitous in combustion systems. These species originate from coal mineral and atmospheric impurities (organic and inorganic), ceramic construction materials, or as additives, such as with potassium seeding for MHD or with bulk glass as a particle absorbing medium. Alkali vapor transport over representative slag, glass, and simple halide, hydroxide and sulfate systems is discussed in relation to materials and process limitations in coal-supported energy systems. Measurement problems associated with vapor transport measurements are also considered.

500,132

PB86-139995

Not available NTIS

National Bureau of Standards (NEL), Boulder, CO. Chemical Engineering Science Div.

Selection of Supports for Immobilized Liquid Membranes.

Final rept.,
J. D. Way, R. D. Noble, and B. R. Bateman. 1985, 10p
Pub. in American Chemical Society Symposium Series n269, St. Louis, Missouri, April 8-13, 1984, Chapter 6, Materials Science of Synthetic Membranes, p119-138 1985.

Keywords: *Membranes, *Supports, Separation, Chemical properties, Molecular structure, Diffusion, Surface chemistry.

Criteria for immobilized liquid membrane (ILM) support selection can be divided into two categories: structural properties and chemical properties. Structural properties include geometry, support thickness, porosity, pore size distribution and tortuosity. Chemical criteria consist of support surface properties and reactivity of the polymer support toward fluids in contact with it. The support thickness and tortuosity determine the diffusional path length, which should be minimized. Porosity determines the volume of the liquid membrane and therefore the quantity of carrier required. The mean pore size determines the maximum pressure difference the liquid membrane can support. The support must be chemically inert toward all components in the feed phase, membrane phase, and sweep or receiving phase.

7C. Organic Chemistry

500,133

PB85-197796

Not available NTIS

National Bureau of Standards (NML), Gaithersburg, MD. Organic Analytical Research Div.

Influence of Substrate Parameters on Column Selectivity with Alkyl Bonded-Phase Sorbents.

Final rept.,
L. C. Sander, and S. A. Wise. 1984, 19p
Pub. in Jnl. of Chromatography 316, p163-181 1984.

Keywords: *Silicon dioxide, *Synthesis (Chemistry), *Polymers, *Sorbents, Substrates, Physical properties, Surface chemistry, Phase rule, Reprints, Chemical reaction mechanisms.

Differences in bonded-phase properties were studied for monomeric and polymeric C18 phases prepared on a variety of silica substrate materials. A total of 22 silicas with pore diameters ranging from 50-1000 Å were used in synthesis. Phase loadings for the resulting bonded phases ranged from 1.3-5.4 micromol/sq m. Physical properties of the substrates including surface area, pore volume, packing density, and background carbon were measured prior to bonding. Large differences were observed in the properties of the silica substrates and in the chromatographic behavior of the resulting phases. Differences in selectivity as well as absolute retention were observed as a function of pore size, with the greatest changes in selectivity occurring for the polymeric phases. The effect of silica pretreatment on phase synthesis and column selectivity was also examined for wide- and narrow-pore substrates. Phases prepared from silica pretreated with acid had greater polymeric character than those prepared from base-pretreated silica. Variation in phase loading and column selectivity is thought to be a function of both the reactivity of the silica surface and pore size. A model for polymeric phase synthesis is proposed where the extent of reaction is limited by a size-exclusion mechanism.

500,134

PB86-129731

PC A03/MF A01

National Bureau of Standards, Gaithersburg, MD. Polymers Div.

Intaglio Ink Considerations.

B. Dickens. Sep 85, 31p NBSIR/85-3216
Sponsored by Bureau of Engraving and Printing, Washington, DC.

Keywords: *Printing inks, *Alkyd resins, *Setting time, *Polymerization, Molecular weight, Solubility, Oxygen, Curing, Thixotropy, Silicon dioxide, Fillers, Performance evaluation.

Alkyds are recommended as the most practical resin system to polymerize in air. The alkyd should have a well-chosen molecular weight distribution and be dispersible in a water-containing solvent system. The sol-

ubility of oxygen in the ink formulations and solvent mixtures should be determined and the compositions adjusted to provide a level of oxygen which gives optimum cure. UV irradiation of the newly printed currency paper can probably be used to skin the ink rapidly and prevent blocking. This may allow printing of both sides of the currency paper in one pass. Replacement of the various pigments and fillers currently in use by dyes attached to the backbone of an organic polymer, either in water-soluble form or in the form of a glass should be investigated. The silica filler may be acting as a desiccant as well as a thickening agent. If this desiccant action is not important, thixotropy of the ink should be adjusted by using sodium carboxy methyl cellulose instead. Other recommendations are given and the formulation of intaglio printing inks is reviewed with special reference to BEP requirements.

7D. Physical Chemistry

500,135

PATENT-4 558 218

Not available NTIS

Department of Commerce, Washington, DC.

Heat Pipe Oven Molecular Beam Source.

Patent,
R. E. Drullinger. Filed 1 Aug 84, patented 10 Dec 85, 7p PB86-137239, PAT-APPL-6-636 769
Supersedes PB85-108132.

This Government-owned invention available for U.S. licensing and, possibly, for foreign licensing. Copy of patent available Commissioner of Patents, Washington, DC 20231 \$1.00.

Keywords: *Molecular beams, *Patents, Sources, Atomic beam sources, Heat pipes, PAT-CL-250-251.

A heat pipe oven molecular beam source wherein a hollow porous metal, metalloid or ceramic body with at least one opening is nearly saturated with the working material and heated to just above the melting point of the working material, generating a thin liquid layer of the working material on the internal surface of the body. Material passing the length of the bore of the body without striking a wall will escape and form the beam. Material striking the liquid layer covering the inside of the body will condense and be conveyed by capillary action back to the closed end of the body.

500,136

PB85-170652

Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

Solubility of Strontianite (SrCO₃) in CO₂-H₂O Solutions between 2 and 91°C, the Association Constants of SrHCO₃⁺(aq) and SrCO₃(sup)(aq) between 5 and 80°C and an Evaluation of the Thermodynamic Properties of Sr²⁺(aq) and SrCO₃(cr) at 25°C and 1 atm Total Pressure.

Final rept.,
E. Busenberg, L. N. Plummer, and V. B. Parker. Oct 84, 15p
Pub. in Geochimica et Cosmochimica Acta 48, p2021-2035 Oct 84.

Keywords: *Solubility, *Strontianite, *Chemical equilibrium, Reprints.

Seventy new measurements (Sr(sub tau)-P(sub CO₂)) of the solubility of strontianite were used to evaluate the equilibrium constant for the reaction SrCO₃(cr) = Sr²⁺(aq) + CO₃²⁻(aq) between 2 and 91°C.

500,137

PB85-172203

Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

Neutron-Induced Reactions and Secondary Ion Mass Spectrometry: Complementary Tools for Depth Profiling.

Final rept.,
G. Downing, R. Fleming, D. Simons, and D. Newbury. 1982, 4p
Pub. in Proceedings of Annual Conference of the Microbeam Analysis Society (17th), Washington, DC., August 9-13, 1982, p219-221.

Keywords: Bismuth, *Secondary ion mass spectroscopy, *Neutron induced reactions, *Depth profiles.

The technique of neutron depth profiling is based upon inducing nuclear reactions by bombardment with low energy neutrons. The nuclear reactions result in the emission of high energy alpha particles or protons. The

energy spectrum of the emitted particles is used to derive a depth distribution by transforming the energy loss into an equivalent depth by stopping power calculations. Depth profiles of bismuth distributions in silicon and tin have been measured by both neutron depth profiling and secondary ion mass spectrometry. Information from both techniques can be used synergistically to aid in a full characterization of the depth distribution.

500,138
PB85-172500 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Intermolecular Potential Calculations for Polycyclic Aromatic Hydrocarbons.
Final rept.,
J. H. Miller, W. G. Mallard, and K. C. Smyth. 11 Oct 84, 8p
Pub. in Jnl. of Physical Chemistry 88, n21 p4963-4970, 11 Oct 84.

Keywords: *Aromatic polycyclic hydrocarbons, *Intermolecular forces, *Potential energy, Soot, Air pollution, Reprints, Benzene, Molecular configuration, Numerical solution, Dimers, Coronene, Circumcoronene.

Methods of calculating the dispersive part of the intermolecular potential for polycyclic aromatic hydrocarbons of D(sub 6h) symmetry are examined. A new, semi-empirical method is utilized to generate the approximate angle dependent dispersive potentials. These dispersive potentials are added to the electrostatic potentials which arise from the permanent quadrupole moments, and the resulting total potential is used to predict the angle between the planes of the molecules in the most stable dimer configuration for the homologous series benzene, coronene, and circumcoronene. These angles are 90, 42, and 36 degrees, respectively, and the well depths at these angles are 2.41, 7.87, and 23.0 kcal/mol.

500,139
PB85-172534 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Chemical Behavior of SO3- and SO5- Radicals in Aqueous Solutions.
Final rept.,
R. E. Huie, and P. Neta. 8 Nov 84, 5p
Sponsored by Department of Energy, Washington, DC.
Pub. in Jnl. of Physical Chemistry 88, n23 p5665-5669, 8 Nov 84.

Keywords: *Free radicals, *Sulfites, *Chemical properties, Solutions, Spectrophotometry, Reaction kinetics, Oxidation, Reprints.

The chemistry of the radicals SO3(-1) and SO5(-1) has been investigated using pulse radiolysis with kinetic spectrophotometry. Rate constants for the oxidation by SO3(-1) of a variety of organic compounds were measured and equilibrium constants determined for the reactions of SO3(-1) with chlorpromazine and phenol. The oxidation of several compounds by SO5(-1) was found to occur more rapidly than their oxidation by SO3(-1). E(SO5(-1)/HSO5(-1)) was estimated to be approximately 1.1V at pH 7.

500,140
PB85-177947 PC A05/MF A01
National Bureau of Standards (NML), Gaithersburg, MD. Center for Analytical Chemistry.
Principles of Quality Assurance of Chemical Measurements.
J. K. Taylor. Feb 85, 81p NBSIR-85/3105

Keywords: *Quality assurance, *Chemical analysis, *Chemical properties, *Measurement, Calibrating, Methodology, Sampling, Inspection, Experimental design, Standards, Standard reference materials.

The general principles of quality assurance of chemical measurements are discussed. They may be classified as quality control -- what is done to control the quality of the measurement process, and quality assessment -- what is done to evaluate the quality of the data output. Quality assurance practices are considered as a hierarchy with levels progressing from the analyst, the laboratory, the project, to the program. The activities of each level are different and depend upon the ones beneath it. Recommendations are presented for developing credible quality assurance practices at each level. An appendix contains outlines that may be used to develop the various documents associated with a quality assurance program.

500,141
PB85-178309 PC A02/MF A01

National Bureau of Standards (NML), Gaithersburg, MD. Center for Analytical Chemistry.

Evaluation of Methods Used for the Determination of Acidity in 'Acid Rain' Samples.
G. Marinenko, and W. F. Koch. Mar 85, 19p NBSIR-85/3114

Sponsored by Environmental Research Center, Research Triangle Park, NC.

Keywords: *Acidity, *Volumetric analysis, *Air pollution, Automation, Performance evaluation, pH, Samples, Ions, *Acid rain, Closed loop systems.

Five methods for the determination of acidity of acid solutions of low concentration (down to .00001 mol/kg) were investigated. Four of the methods provide satisfactory results. Method (3), Gran's plot end-point detection using .001 M NaOH titrant, suffers from the inability to control exactly the size of reagent increments, which is essential for this method. Automated titration systems could remedy this deficiency.

500,142
PB85-179075 (Order as PB85-179042, PC A06/MF A01)
National Bureau of Standards, Gaithersburg, MD. Center for Materials Science.

Interactions of Composition and Stress in Crystal-line Solids.

F. C. Larche, and J. W. Cahn. 30 Aug 84, 34p
Prepared in cooperation with Montpellier-2 Univ. (France).
Included in Jnl. of Research of the National Bureau of Standards, v89 n6 p467-500 Nov-Dec 84.

Keywords: *Crystals, *Stress analysis, *Solids, Phase transformation, Thermodynamics.

The thermodynamics of stressed crystals that can change phase and composition is examined with particular attention to hypotheses used and approximations made. Bulk and surface conditions are obtained and for each of them practical expressions are given in terms of experimentally measurable quantities. The concept of open-system elastic constants leads to the reformulation of internal elastochemical equilibrium problems into purely elastic problems, whose solutions are then used to compute the composition distribution. The atmosphere around a dislocation in a cubic crystal is one of several examples that are completely worked out. The effects of vacancies and their equilibrium within a solid and near surfaces are critically examined, and previous formulas are found to be first order approximations. Consequences of the boundary equations that govern phase changes are studied with several examples. Finally, problems connected with diffusional kinetics and diffusional creep are discussed.

500,143
PB85-179091 (Order as PB85-179083, PC A05/MF A01)

National Bureau of Standards, Gaithersburg, MD.
Development of a One-Micrometer-Diameter Particle Size Standard Reference Material.

G. W. Mulholland, A. W. Hartman, G. G. Hembree, E. Marx, and T. R. Lettieri. 11 Oct 84, 24p
Included in Jnl. of Research of the National Bureau of Standards, v90 n1 p3-26 Jan-Feb 85.

Keywords: *Particle size, *Standards, *Polystyrene, Light scattering, Optical measurement, Spheres, Surfaces, Error analysis, Mic scattering, *Standard reference materials, Transmission electron microscopy.

The average diameter of the first micrometer particle size standard (Standard Reference Material 1690), an aqueous suspension of monosized polystyrene spheres with a nominal 1 micrometer diameter, was accurately determined by three independent techniques. In one technique the intensity of light scattered by a diluted suspension of polystyrene spheres was measured as a function of scattering angle, using a He-Ne laser polarized in the vertical direction. The second technique consisted of measuring as a function of angle the intensity of light scattered from individual polystyrene spheres suspended in air, using a He-Cd laser with light polarized parallel and perpendicular to the scattering plane. The measurement of row length by optical microscopy for polystyrene spheres arranged in close-packed, two-dimensional hexagonal arrays was the basis of the third technique. The measurement errors for each technique were quantitatively assessed. For the light scattering experiments, this required simulation with numerical experiments. The average diameter determined by each technique agreed within 0.5% with the most accurate value being 0.895

+ or - 0.007 micrometers based on light scattering by an aqueous suspension. Transmission electron microscopy, flow through electrical sensing zone counter measurements, and optical microscopy were also used to obtain more detailed information on the size distribution including the standard deviation (0.0095 micrometers), fraction of agglomerated doublets (1.5%).

500,144
PB85-179109 (Order as PB85-179083, PC A05/MF A01)
National Bureau of Standards, Gaithersburg, MD.

Stable Law Densities and Linear Relaxation Phenomena.

M. Dishon, G. H. Weiss, and J. T. Bendler. 27 Nov 84, 13p

Prepared in cooperation with National Institutes of Health, Bethesda, MD., and General Electric Corporate Research and Development, Schenectady, NY.
Included in Jnl. of Research of the National Bureau of Standards, v90 n1 p27-39 Jan-Feb 85.

Keywords: *Density(Mass/volume), *Molecular relaxation, *Mathematical models, *Linearity, Polymers, Semiconductors, Tables(Data), Stability, Numerical solution.

Stable law distributions occur in the description of the linear dielectric behavior of polymers, the motion of carriers in semi-conductors, the statistical behavior of neurons, and many other phenomena. No accurate tables of these distributions or algorithms for estimating the parameters in these relaxation models exist. In this paper the authors present tables of the functions together with related functional properties of $zQ(\text{sub } \alpha)$ (z). These are useful in the estimation of the parameters in relaxation models for polymers and related materials. Values of the integral $Q(\text{sub } \alpha)$ (z) are given for $\alpha=0.01, 0.02(0.02)0.1(0.1)1.0(0.2)2.0$ and those of $V(\text{sub } \alpha)$ (z) are given for $\alpha=0.0(0.1)0.1(0.1)2.0$. A variety of methods was used to obtain six place accuracy. The tables can be used to sequentially estimate the three parameters appearing in the Williams-Watts model of relaxation. An illustration of this method applied to data in the literature is given.

500,145
PB85-182715 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.

Far Infrared Absorption in Normal H2 from 77 K to 298 K.

Final rept.,
P. Dore, L. Nencinini, and G. Birnbaum. 1983, 9p
Pub. in Jnl. of Quantitative Spectroscopy and Radiative Transfer 30, n3 p245-253 Sep 83.

Keywords: *Hydrogen, Absorption, Molecular rotation, Temperature, Reprints, *Far infrared spectroscopy.

The translational-rotational absorption spectrum of normal H2 has been measured from 80 to 900/cm at seven temperatures from 77.4 to 298 K. These results have been accurately fitted by a three parameter line shape function thereby providing a reliable way of predicting the absorption of H2 anywhere in this frequency and temperature region.

500,146
PB85-182731 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.

Diamagnetism in Excited States of Hydrogen.

Final rept.,
C. W. Clark, and K. T. Taylor. 1982, 9p

Sponsored by North Atlantic Treaty Organization.
Pub. in Jnl. Phys.Colloq. 43, n2 p127-135 Nov 1982.
Meeting on Atomic and Molecular Physics Close to Ionization Thresholds in High Fields, Aussois, France, June 7-11, 1982.

Keywords: *Magnetic fields, *Diamagnetism, Experimental design, Excitation, Zeeman effect, Ionization, Forecasting, Reprints, *Hydrogen atoms, *Rydberg series, Numerical solution.

The spectrum of high Rydberg states of atomic hydrogen in a magnetic field has received much attention in the last few years. Although no experimental work has been done, theoretical activity has elucidated major features of the spectrum ranging in energy up to a few cyclotron frequency units below the ionization threshold. In the weak field limit an unexpected richness of structure has been uncovered by perturbative treatments based on the 0(4) symmetry of hydrogen.

Field 7—CHEMISTRY

Group 7D—Physical Chemistry

Though this symmetry is absent in the more complex atoms for which experimental data are available, the authors believe that a comprehensive theory of Rydberg diamagnetism will ultimately be phrased in hydrogenic language. The authors review here the basic physics which motivates this hypothesis, the experimental and numerical results which substantiate it, and the opportunities it suggests for future investigations.

500,147

PB85-182756

Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

Sputter Coated Carbon Specimens for SEM Performance Testing.

Final rept.,

D. R. Black, and D. B. Ballard. 1982, 2p

Sponsored by Electron Microscopy Society of America, Oak Ridge, TN.

Pub. in Proceedings of Annual Meeting on Electron Microscopy Society of America (40th), Washington, DC. August 9-13, 1982, p750-751.

Keywords: *Carbon fibers, *Metal coatings, Performance evaluation, Sputtering, Substrates, Graphitizing, *Scanning electron microscopy.

A performance test is recommended as a supplement to the image separation resolution determination for the SEM. The performance test involves measurement of the straight line (slope) segment of a step waveform in a specified manner divided by the known magnification. Two different carbon substrates sputter etched, then sputter coated with Au-Pd were developed that provide the necessary electron beam-specimen edge profile for wave-form analysis. One substrate is a spectrographic grade carbon disc and the other is graphitized polymer fibers.

500,148

PB85-182764

Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

Thermoneutral Isotope Exchange-Reactions of Cations in the Gas-Phase.

Final rept.,

P. Ausloos, and S. G. Lias. 1981, 7p

Pub. in Jnl. of the American Chemical Society 103, n13 p3641-3647 1981.

Keywords: *Cations, *Vapor phases, *Isotope exchange, *Reaction kinetics, Chemical reactions, Reprints, *Ion molecule interactions.

Rate constants have been measured for reactions of the type: $RD(+1) + MH \rightarrow RH(+1) + MD$ where $RD(+1)$ is CD_3CND , $CD_3CDOD(+1)$, $CD_3CODCD(+1)3$, or $(C_2D_5)2OD+$ and the MH molecules are alcohols, acids, mercaptans, H_2S , AsH_3 , PH_3 , or aromatic molecules. Rate constants are also presented for the reactions: $Ar(sub H)D(+1) + D(sub 2)O \rightarrow Ar(sub D)D(+1)$ is a deuterated aromatic molecule and $Ar(sub D)D(+1)$ is the same species with a D atom incorporated on the ring. In all but two cases, the competing deuterium transfer is sufficiently endothermic that it can not be observed under the conditions of the ICR experiments at 320-520 K.

500,149

PB85-182806

Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

Elastic and Inelastic Scattering of Electrons by Atomic-Hydrogen at Intermediate Energies in a Coupled-Channel Second Order Potential Model.

Final rept.,

B. H. Bransden, T. Scott, R. Shingal, and R. K.

Roychoudhury. 1982, 12p

Pub. in Jnl. of Physics B: Atomic and Molecular Physics 15, n24 p4605-4616 1982.

Keywords: *Elastic scattering, *Inelastic scattering, *Electron scattering, *Mathematical models, Excitation, Reprints, *Hydrogen atoms.

A second-order model employing a pseudostate expansion in intermediate states is applied in a 1s-2s-2p coupled channel formalism to electron scattering by atomic hydrogen in the energy range 54 to 200 eV. Although the model predicts cross sections for elastic scattering, and excitation of the $n = 2$ levels, which are in reasonable accord with the experimental data, the predicted results for the angular correlation parameters show little improvement over the 1s-2s-wp close coupling model.

500,150

PB85-182814

Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

Auger Electron Emission from the Decay of Collisionally-Excited Atoms Sputtered from Al and Si.

Final rept.,

T. D. Andreadis, J. Fine, and J. A. D. Matthew. 1983,

8p

Sponsored by Centre National d'Etudes des Telecommunications, Lannion (France), and CEA Centre d'Etudes Nucleaires de Grenoble (France), Lab. d'Electronique et de Technologie de l'Informatique.

Pub. in Proceedings of International Conference on Ion Beam Modification of Materials (3rd), Grenoble, France, September 6-10, 1982, Nuclear Instruments and Methods in Physics Research, 209-210, p11 p495-502, 1 May 83.

Keywords: *Aluminum, *Silicon, *Auger electrons, *Ion beams, *Ion irradiation, Sputtering, Monte Carlo method, Solids, Reprints, *Atom atom interactions, *Auger spectroscopy.

Atom collisions of several keV may result in inner-shell excitations. The energy spectra of Auger electrons from excitations induced by ion bombardment of solid materials are different from those stimulated by x-rays or electrons. Auger electron spectra produced by ion bombardment of solids contain features similar to spectra obtained from atoms undergoing Auger transitions in the gas phase, i.e., atomic-like spectra. An interpretation of the atomic-like spectra from ion-bombarded solids is that a significant portion of the atoms undergoing Auger de-excitation have previously been sputtered from the solid. Auger decay in the gas phase can occur if the inner-shell lifetime is sufficiently long for the excited atom to escape. Results from our Monte Carlo calculations of the origin, movement, and decay of ion-bombardment induced 2p inner-shell excitations of Al and Si will be presented. These calculations indicate that a significant portion of the Auger emission originates from sputtered atoms; the kinetic energy of atoms sputtered while experiencing inner-shell excitation far exceeds the average kinetic energy of sputtered atoms, and so, Auger electron emission may constitute a probe of the high energy collision cascade near the surface. Calculated dependence of the Auger electron intensity on the incident angle of the ion beam will be compared with measurements, and the effect of inner-shell lifetime on the calculated Auger electron intensity will be discussed.

500,151

PB85-182855

Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

Critical Evaluation of Thermodynamic Data: A Research Activity.

Final rept.,

S. Abramowitz, D. D. Wagman, V. B. Parker, and D.

Garvin. 1984, 12p

Pub. in NATO Adv. Study Inst. Ser., Ser. C 119, p803-814 1984.

Keywords: *Thermodynamics, *Research projects, Tables(Data), Reprints, Computer applications.

The principles underlying the evaluation of thermodynamic data are described. The role of modern computer technology in data evaluation is discussed.

500,152

PB85-182863

Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

Barriers to Internal Rotation in Inorganic Species.

Final rept.,

S. Abramowitz. 1984, 14p

Pub. in NATO Adv. Study Inst. Ser., Ser. C 119, p789-802 1984.

Keywords: *Inorganic compounds, *Molecular rotation, *Infrared spectroscopy, *Raman spectroscopy, *Barriers, Thermodynamics, Molecular vibration, Reprints.

Barriers to internal rotation have been determined using infrared and Raman spectroscopy for some inorganic species. The determination of these barriers will be described for a high barrier (BCl_2SH) a medium barrier (PF_5 , AsF_5 and VF_5) and a low or zero energy barrier ($B(CH_3)_3$).

500,153

PB85-182905

Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

Oxidation of the Ti(0001) Surface.

Final rept.,

E. Bertel, R. Stockbauer, and T. E. Madey. 1983, 2p

Pub. in Jnl. of Vacuum Science and Technology, A1 n2 p1075-1076 1983.

Keywords: *Surface chemistry, *Oxidation, *Titanium, *Electronic spectra, Titanium oxides, Reprints.

Upon exposure of a Ti(0001) surface to oxygen a thin oxide overlayer is formed as revealed by ELS. AES, UPS, and ESD indicate a TiO_2 stoichiometry in this surface oxide.

500,154

PB85-183192

Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

Multiple Reflection Corrections in Fourier Transform Spectroscopy.

Final rept.,

A. Baghdadi. 1983, 10p

Sponsored by Electrochemical Society, Inc., Pennington, NJ. Electronics Div.

Pub. in Proceedings of a Symposium on Defects in Silicon, San Francisco, CA., May 8-13, 1983, Proc. Electrochem. Soc. 83, n9 p293-302 1983.

Keywords: *Infrared spectroscopy, *Surfaces, *Fourier transform spectroscopy.

In order to account properly for multiple passes of the infrared beam in back-surface damaged wafers in infrared spectrometers, the effective reflectivity of the back surface must be measured. Two methods for accomplishing this are evaluated in a comparative study. The first method is based upon an analysis of the spectrum and the second method is based upon an analysis of the interferogram.

500,155

PB85-183218

Not available NTIS

National Bureau of Standards (NML), Gaithersburg, MD. Molecular Spectroscopy Div.

Summary of Group Theoretical Results for Microwave and Infrared Studies of H₂O₂.

Final rept.,

J. T. Hougen. Jun 84, 11p

Pub. in Canadian Jnl. of Physics 62, n12 p1392-1402 Jun 84.

Keywords: *Hydrogen peroxide, *Molecular rotation, *Microwave spectroscopy, *Infrared spectroscopy, Reprints.

Group theoretical treatments found in the literature for other molecules, based on double-groups of appropriate permutation-inversion groups, are modified slightly and applied to H_2O_2 . This permits a more unified view of many theoretical results derived in various earlier studies of the molecule. Briefly, if no effects due to internal rotation tunneling were observed in the H_2O_2 spectrum, the molecule could be treated using the C_2 point group of its equilibrium geometry. If effects due to internal rotation tunneling were observed in the trans barrier are observed (as is presently the case), the molecule should be treated using the C_{2h} point group of its trans planar conformation at the top of the tunneling barrier. An empirically discovered successful fitting procedure for the ground state rotational levels, reported in a treatment of microwave and millimeter wave measurements on H_2O_2 , can be rationalized on the basis of the present theoretical results.

500,156

PB85-183226

Not available NTIS

National Bureau of Standards (NML), Gaithersburg, MD. Chemical Kinetics Div.

Vinylidene (3B2): An Active Intermediate in the Photolysis of Ethylene.

Final rept.,

A. H. Laufer. 1984, 5p

Sponsored by National Aeronautics and Space Administration, Washington, DC.

Pub. in Jnl. of Photochemistry 27, p267-271 1984.

Keywords: *Vinylidene resins, *Photolysis, *Ethylene, *Ultraviolet spectroscopy, Excitation, Photochemistry, Reprints.

Triplet vinylidene has been observed, by time-resolved absorption spectroscopy, as an intermediate in the vacuum UV flash photolysis of ethylene. The several primary photochemical processes are discussed. Rate constants for the interaction of both protonated and deuterated vinylidene species with C_2H_4 and C_2D_4 have been obtained. The nature of the interaction between triplet vinylidene and ethylene is discussed.

500,157

PB85-183242

Not available NTIS

National Bureau of Standards (NEL), Gaithersburg, MD. Thermophysics Div.

Thermal Expansion Coefficient of FCC Metals.

Final rept.,
R. A. MacDonald. 1984, 9p
Pub. in Thermal Expansion 8, p11-19 1984.

Keywords: *Thermodynamic properties, *Thermal expansion, Forecasting, Reprints.

The work to be reported here improves upon and extends that presented at the 7th European Thermophysical Properties Conference in 1980. There it was shown that the calculated thermal expansion values, epsilon, were very sensitive to the curvature of the potential, phi (r), assumed for the nearest neighbor interaction. The authors give a brief summary of the theory pertinent to their calculation of the thermodynamic properties of the fcc metals. Next they present the results that were obtained for the thermal expansion of copper and then they examine the problem of obtaining alpha by derivation from thermal expansion data. They find that there can be quite a large variation in the values of alpha derived from thermal expansion data and they urge that the 'direct' method of measurement of alpha be used in the future.

500,158

PB85-183267

Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.

Planar Ca-PO₄ Sheet-Type Structures: Calcium Bromide Dihydrogenphosphate Tetrahydrate, CaBr(H₂PO₄)-4H₂O, and Calcium Iodide Dihydrogenphosphate Tetrahydrate, CaI(H₂PO₄)-4H₂O.

Final rept.,
M. Mathew, S. Takagi, and W. E. Brown. 1984, 4p
Sponsored by American Dental Association Health Foundation, Chicago, IL.
Pub. in Acta Crystallographica C40, p1662-1665 1984.

Keywords: *Calcium phosphates, *Crystal structure, Sheets, Reprints.

Both compounds have planar sheet-type structures consisting of Ca-H₂PO₄ chains. The halide ions, X, and the water molecules are linked via O-H...X hydrogen bonds to form X(H₂O)₆ octahedra. These octahedral units are linked together to form a polymeric layer (X(H₂O)₄)_n between the Ca-H₂PO₄ sheets.

500,159

PB85-183317

Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD.

Inelastic Mean Free Paths and Attenuation Lengths of Low-Energy Electrons in Solids.

Final rept.,
C. J. Powell. 1984, 16p
Pub. in Scanning Electron Microscopy IV, p1649-1664 1984.

Keywords: *Surface chemistry, *Solids, *Electron energy, Dielectric properties, Free electron theory, Reprints.

Calculations of inelastic mean free paths and measurements of attenuation lengths of low-energy electrons in solids have been studied. The emphasis of the study was on the systematics of the dependences of these quantities on material and electron energy. Calculations of inelastic mean free paths from experimental dielectric data indicate that different dependences on electron energy occur in different materials and that deviations from simple theoretical or empirical expressions are to be expected.

500,160

PB85-183390

PC A03/MF A01
National Bureau of Standards (NML), Gaithersburg, MD. Chemical Thermodynamics Div.

GAMPHI - A Database of Activity and Osmotic Coefficients for Aqueous Electrolyte Solutions.

Technical note,
R. N. Goldberg, J. L. Manley, and R. L. Nuttall. Mar 85, 28p NBS/TN-1206
Also available from Supt. of Docs as SN003-003-02640-9. Sponsored by Department of Energy, Pittsburgh, PA.

Keywords: *Information systems, *Activity coefficients, *Osmosis, *Electrolytes, Fortran, Thermodynamics, Solutions, Computer programming, Gibbs free energy.

A database of activity and osmotic coefficients for 350 binary aqueous electrolyte solutions at 298.15 K has

been assembled together with a collection of subroutines for utilizing the database. The computer codes, which are written in FORTRAN 77, can be used either interactively or from user-written programs to calculate values of the activity and osmotic coefficients at selected molalities.

500,161

PB85-183515

Not available NTIS
National Bureau of Standards, Gaithersburg, MD.

Validation of the Sulfur Concentration of Selected Iron-Base NBS (National Bureau of Standards) Standard Reference Materials by Isotope Dilution Spark Source Mass Spectrometry.

Final rept.,
R. W. Burke, P. J. Paulsen, E. J. Maienthal, and G. M. Lambert. 1982, 5p
Pub. in Talanta 29, n10 p809-813 1982.

Keywords: *Chemical analysis, *Sulfur, *Iron containing alloys, Concentration(Composition), Equilibrium, Reprints, *Standard reference materials, *Isotopic dilution spark source mass spectrometry.

An isotopic dilution spark source mass spectrometric procedure has been developed for the accurate determination of sulfur in iron-base alloys. A sealed tube dissolution technique is used to prevent volatilization losses and to effect isotopic equilibration. Application of this technique to the reanalysis of existing NBS Standard Reference Materials yields results that are generally in good agreement with the certified values.

500,162

PB85-183549

Not available NTIS
National Bureau of Standards, Gaithersburg, MD.

Detection of the 2p¹ Orbital of CO and NO Chemisorbed on Ni(111) by Surface Penning Ionization Electron Spectroscopy (SPIES).

Final rept.,
F. Bozso, J. Arias, J. T. Yates, R. M. Martin, and H. Metiu. 1983, 4p
Pub. in Chemical Physics Letters 94, n3 p243-246 1983.

Keywords: *Carbon monoxide, *Nitrogen oxides(NO), *Chemisorption, Nickel, Surface chemistry, Ionization, Reprints, *Surface Penning Ionization Electron Spectroscopy.

The authors use surface Penning ionization spectroscopy (SPIES) to study the electronic properties of CO and NO adsorbed on Ni(111). In this experiment an atomic beam containing ground state and 2 singlet S He atoms collides with the adsorbate covered Ni(111) surface. This causes the transfer of approximately 20.6 eV energy into the electronic degrees of freedom of the adsorbate molecules, forcing them to emit electrons. The SPIE spectrum is obtained by analyzing the energy of these electrons. The high surface sensitivity of this method allows us to measure the binding energy of the partly filled 2p¹ orbitals of CO and NO.

500,163

PB85-184521

Not available NTIS
National Bureau of Standards, Gaithersburg, MD.

Analyses of the Aqueous Phase During Early C3S Hydration.

Final rept.,
P. W. Brown, E. Franz, G. Frohnsdorff, and H. F. W. Taylor. 1984, 6p
Pub. in Cement and Concrete Research 14, n2 p257-262 1984.

Keywords: *Liquid phases, *Hydration, Surfaces, Reprints, *Carbon sulfide, Phase equilibrium.

The concentrations of calcium and silica in solution during the first 4 hours of C3S hydration were measured. The results of these analyses indicate that a solid hydrate forms within 30 seconds of hydration and that an equilibrium between the solution and the solid hydration product is rapidly established. A strong dependence of the degree of early hydration on the water to C3S ratio was observed, while the dependence on the surface area of the C3S was minimal.

500,164

PB85-184547

Not available NTIS
National Bureau of Standards, Gaithersburg, MD.

Effects of Coherency Constraints on Phase Equilibria.

Final rept.,
J. W. Cahn, and F. C. Larche. 1983, 2p
Sponsored by Materials Research Society, University Park, PA., and American Society for Metals, Metals Park, OH.

Pub. in Proceedings of Symposium on Alloy Phase Diagrams, Boston, MA., November 1982, Materials Research Society Symposia Proceedings, v19 p311-312 1983.

Keywords: *Thermodynamics, Alloys, Phase diagrams, Congruencies, Consolidation, Strain energy methods, *Phase equilibrium, Solid state chemistry.

The thermodynamics of coherent phase equilibria is reviewed. It is recommended that boundaries between fields in which different combinations of phases coexist coherently be depicted on phase diagrams. However, the compositions of coexisting phases cannot be read from such a diagram because tie-lines will not usually end on these boundaries. Apparent discrepancies between different experimental phase diagram determination for solid state equilibria may have a sound physical basis.

500,165

PB85-184562

Not available NTIS
National Bureau of Standards, Gaithersburg, MD.

Polymer Crystallization: Proper Accounting of a Wider Class of Paths to Crystallization Variations on a Theme of Point.

Final rept.,
E. A. Di Marzio, and C. M. Guttman. 1982, 10p
Pub. in Jnl of Applied Physics 53, n10 p6581-6590 Oct 82.

Keywords: *Crystallization, *Polymers, Crystal growth, Nucleation, Reprints, Monomers.

Point has suggested that during the polymer crystallization process individual stems form by zippering of monomer segments onto the substrate and that at any time during the zippering process the stem can fold over, thus initiating a new stem. The authors augment the treatment of Point analytically by allowing each of the subsequent stems to fold any stage in the zippering process rather than only during the forming of the first stem. The problem is isomorphic to the mathematical problem of the growth of a Cayley Tree with infinite branching. Although there is net growth, the rules of growth (crystallization) are such that branches of the tree can be resorbed. By use of a simple renormalization technique, formulae are obtained both for the steady state growth rate and for the lamellar thickness which for special cases reduce to the Point results. Classical nucleation theory remains valid at low to moderate supercoolings.

500,166

PB85-184604

Not available NTIS
National Bureau of Standards, Gaithersburg, MD.

Cross Polarization-Magic Angle Sample Spinning NMR Study of Several Crystal Forms of Lactose.

Final rept.,
W. L. Earl, and F. W. Parrish. 1983, 10p
Pub. in Carbohydrate Research 115, n1 p23-32 1983.

Keywords: *Isotopic labeling, *Lactose, *Nuclear magnetic resonance, *Molecular structure, Carbon 13, Reprints, *Chemical shifts(Nuclear magnetic resonance).

Five different crystalline forms of lactose were investigated using cross polarization-magic angle sample spinning (13)C (CP-MAS) NMR. Both the anhydrous beta-lactose and the alpha-lactose monohydrate structures are known from x-ray diffraction studies and the CP-MAS NMR data agree with those structures. The structure of the stable anhydrous alpha-lactose has not been reported. The CP-MAS NMR results indicate that the crystal must have two or more lactose molecules per unit cell. The chemical shifts measured for two mixed crystals with alpha:beta ratios of 5:3 and 4:1 are a direct result of the fact that both materials are real mixed crystals rather than physical mixtures of crystals of pure alpha- and beta-lactose. The chemical shifts also indicate that the lactose molecules in both mixed crystals are in environments similar to the crystalline environment of the stable anhydrous alpha-lactose.

500,167

PB85-184612

Not available NTIS
National Bureau of Standards, Gaithersburg, MD.

Thermochemistry of Interface and Surface Segregation and Chemisorption for Core Level Binding Energy Shifts.

Final rept.,
W. F. Egelhoff. 1983, 2p
Pub. in Jnl. of Vacuum Science and Technology 1, n2 p1102-1103 Apr/Jun 83.

Field 7—CHEMISTRY

Group 7D—Physical Chemistry

Keywords: *Thermochemistry, *Surface chemistry, *Interfaces, *Copper, *Carbon monoxide, Chemisorption, Nickel, Binding, Reprints.

The equivalent core approximation has been applied to measured shifts in core level binding energies to determine thermochemical values. The examples reported here are, first the heat of interface segregation for Cu in bulk Ni to a Cu-Ni interface, second the heat of surface segregation of Cu to a Ni surface and third the difference in the heat of CO chemisorption on Cu and Ni.

500,168
PB85-184653 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Measurement of Ionization Rates of Ti IX, Ne VI, Ne VII and O VI.
Final rept.,
R. U. Datla, and J. R. Roberts. 1983, 8p
Sponsored by Department of Energy, Washington, DC.
Office of Fusion Energy.
Pub. in Physics Review A: General Physics 28, n4 p2201-2208 Oct 83.

Keywords: *Ionization, *Reaction kinetics, *Titanium, *Neon, *Oxygen, Reprints, *Plasma spectroscopy, *Electron ion interactions.

The effective ionization rates of Ti IX, Ne VI, Ne VIII and O VI have been measured using the plasma spectroscopy method in a theta-pinch discharge at an electron temperature (50-60 eV) much below their ionization threshold and at an electron density of (about 2-3) 10^{16} to the 16th power/cm³. A theoretical analysis of the effective ionization rates showed that excitation-ionization is a major contributing process. Theoretical values are in reasonable agreement with experiment.

500,169
PB85-184687 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Enskog Theory for Multicomponent Mixtures: 1. Linear Transport Theory.
Final rept.,
M. L. de Haro, E. G. D. Cohen, and J. M. Kincaid. 1983, 14p
Pub. in Jnl. of Chemical Physics 78, n5 p2746-2759, 1 Mar 83.

Keywords: *Transport theory, *Fluids, Mixtures, Viscosity, Thermal conductivity, Diffusion coefficients, Reprints, *Enskog-Thome theory.

The Enskog theory for dense multicomponent fluid mixtures is developed. Two versions are considered: the standard theory and the revised theory. Explicit expressions for all the transport coefficients (shear and bulk viscosity, thermal conductivity, mutual and thermal diffusion coefficients) in terms of the sizes, masses, and concentrations of the constituents of the mixture are given in third Enskog approximation. Applications will be discussed in subsequent papers.

500,170
PB85-184695 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Multi-Vacancy Effects in Argon K-Spectra.
Final rept.,
R. D. Deslattes, P. L. Cowan, R. E. LaVilla, and K. Dyall. 1982, 5p
Sponsored by National Science Foundation, Washington, DC.
Pub. in Proceedings of International Conference on X-Ray and Atomic Inner-Shell Physics, 'X-82', Eugene, OR., August 23-27 1982, AIP Conference Proceedings n94, p100-104.

Keywords: *Argon, *Atomic energy levels, *X-ray analysis, Emission spectroscopy, Excitation.

The authors have carried out coordinated measurements of K series emission and absorption spectra in atomic argon. Specifically, emission spectra (especially in the region of K(beta_{sub 1,3})) were recorded with photon excitation energies ranging from below the single-vacancy threshold to energies above most important double-vacancy thresholds. Satellite emission spectra were modelled using both Dirac-Fock and Configuration Interaction (CI) calculations. Comparisons with experiment show reasonable agreement of the CI calculations for the first high energy satellite complex, beta_{sub 1}(sup V), but not for the second, beta_{sub 2}.

500,171
PB85-184729 Not available NTIS

National Bureau of Standards, Gaithersburg, MD.
Preface to Industrial Applications of Surface Analysis.
Final rept.,
L. A. Casper, and C. J. Powell. 1982, 2p
Sponsored by American Chemical Society, Washington, DC.
Pub. in Proceedings of Symposium of the American Chemical Society (181st), New York, August 23-28, 1981, ACS Symposium Series 199, pvii-viii, 1982.

Keywords: *Surface analysis, *Industrial plants, Interfaces.

This paper is the Preface for a book which contains the Proceedings of a Symposium on Industrial Application of Surface Analysis held at the 181st American Chemical Society National Meeting, New York, NY, August 23-28, 1981. The Preface describes briefly the significance of surface analysis in industry and the scope and purpose of the Symposium.

500,172
PB85-184760 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Application of Hueckel-Moebius Concept to Torsional Vibration and Internal Rotation of Molecules.
Final rept.,
Y. N. Chiu. 1984, 18p
Pub. in Theochem 17, n3-4 p211-228 Apr 84.

Keywords: *Molecular rotation, *Molecular vibration, Angular momentum, Ethane, Reprints, *Huckel molecular orbitals, *Huckel approximation, *Linear combination of vibrational wavefunctions.

Linear combination of vibrational wavefunctions (LCVW) centered at the periodic potential minima is used to represent the approximate torsional wavefunction of the hindered internal rotation of a coaxial (XY(sub n))₂-type molecule. These linear combinations are shown to have the correct pseudo-angular momentum upon rotation of one or both parts of the rotor. And they are uniquely correlated with the wavefunctions of free internal rotation having the same angular momentum.

500,173
PB85-184778 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Neutron Diffraction Study of Sodium Sesquicarbonate Dihydrate.
Final rept.,
C. S. Choi, and A. D. Mighell. 1982, 3p
Pub. in Acta Crystallographica, Section B: Structural Crystallography and Crystal Chemistry 38, n11 p2874-2876, 15 Nov 82.
Keywords: *Crystal structure, *Neutron diffraction, *Hydrogen bonds, Least squares method, Sodium carbonates, Reprints, *Sodium sesquicarbonate dihydrate.

Na₂CO₃:NaHCO₃:2H₂O, M(sup r) = 220.0, monoclinic, C2/c, a = 20.36(2), b = 3.48(1), c = 10.29(1) Å, beta = 106.48(1) degrees, Z = 4, Dx = 2.147 Mg/cm³. The final R value after full matrix least-squares refinement was 0.040 for 932 observed reflections. Analysis of thermal ellipsoids and least-squares refinement of a split hydrogen model reveal that this hydrogen atom may be viewed as slightly disordered.

500,174
PB85-184786 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
SEM and TEM Investigation of Sintering in Anorthite.
Final rept.,
L. P. Cook. 1982, 18p
Sponsored by Metallurgical Society of AIME, Warrendale, PA., and American Ceramic Society, Columbus, OH. Basic Science Div.
Pub. in Proceedings of Symposium on Metal and Ceramic Powders, Louisville, KY., October 12-14, 1981, Processing of Metal and Ceramic Powders, p165-182, 1982.

Keywords: *Densification, *Sintering, *Kinetics, Diffusion, Powders, *Anorthite, *Scanning electron microscopes, *Transferred electron microscopes, Calcium aluminate silicate.

By comparison with other tectosilicates, powdered crystalline anorthite (CaAl₂Si₂O₈) shows a strong tendency for densification during sintering. Experi-

ments have been conducted to determine the conditions under which this behavior is reproducible and to determine the mechanism or mechanisms responsible. Results indicate that while minor changes in grain size distribution have a large effect upon the kinetics of sintering and densification, relatively coarse powders ultimately yield as dense a product as powders with a much higher percentage of fines. A two-stage hypothesis for densification at 1400C is proposed: (1) an early rapid densification associated with grain boundary diffusion driven by minimization of highly anisotropic surface energy; (2) volume diffusion, primarily along closely spaced parallel twin planes.

500,175
PB85-187268 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Number and Novelty in Approaches to the Calculation of Strainless Group Increments.
Final rept.,
D. Van Vechten, and J. F. Liebman. 1981, 6p
Pub. in Israel Jnl. of Chemistry 21, n2-3 p105-110 1981.

Keywords: *Strain energy methods, *Molecular structure, *Thermochemistry, Differences, Reprints, *Alicyclic hydrocarbons.

In this paper, the authors show that the large number of approaches using apparently unrelated strainless increments for unsubstituted alicyclic hydrocarbons in the literature are neither mathematically nor conceptually unique. They additionally demonstrate that if the strain energy assigned to a compound by any three sets of increments are known, the strain energy any other approach would assign can automatically be determined without considering any further details of the structure of the compound. Equivalently, there are but three mathematically distinct, i.e. linearly independent, strainless incremental approaches for these compounds. Thus the choice of which method to employ in one's own reasoning relative to a chemical problem must be based on personal, rather than strictly chemical or mathematical criteria. They proceed by presenting our criteria and their molecular realization, the concepts of diagonal reference states. Diagonal reference states are defined from hydrocarbons composed solely of the group of interest. The virtues and debits of this method are presented in support of their conclusion that this approach is preferable because it is diagonal.

500,176
PB85-187276 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Inferences About Molecular Motion from Proton Decoupled ¹³C NMR Spectra of Solid Polymers.
Final rept.,
D. L. Vanderhart, G. G. A. Bohm, and V. D. Mochel. 1981, 1p
Pub. in Abstracts of Papers American Chemical Society 182, 112p Aug 81.

Keywords: *Nuclear magnetic resonance, *Solids, *Polyethylene, *Polyethylene terephthalate, *Molecular rotation, Carbon 13, Mechanical properties, Magnetic fields, Sites, Comparison, Reprints, *Chemical shifts(Nuclear magnetic resonance).

Proton decoupled (¹³C) spectra are used to describe molecular motion in polyethylene (PE) and polyethyleneterephthalate (PET). Use of static oriented samples suitably aligned in the magnetic field allow one to obtain information about the frequency and geometry of motion from the (¹³C) lineshape. In systems with appropriate symmetries, molecular motion can effect an exchange between magnetically inequivalent sites. In particular, 180 degrees flip-flop motions in the crystalline regions of PE and aromatic ring flip-flops in PET represent two-site exchange processes with equal populations at each site. The dipolar interaction between isolated pairs of (¹³C) nuclei was used to study flip-flop motions in PE whereas the anisotropic chemical shift of the protonated aromatic carbons in PET was used to study aromatic ring motion. For the flip-flop motion in crystalline PE comparison will be made with some dynamic mechanical measurements. It is felt that information about crystalline motions is generalizable to unoriented, melt crystallized samples since some of the oriented samples were annealed so as to minimize any crystalline defects introduced by mechanical deformation.

500,177

PB85-187292 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Photoionization of Liquid Benzene: Fluorescence and Electron Scavenger Quenching between 1900 and 1150-A.
Final rept.,
F. P. Schwarz, and M. Mautner. 1982, 6p
Pub. in Chemical Physics Letters 85, n2 p239-244 1982.

Keywords: *Photochemical reactions, *Ionization, *Ultraviolet spectroscopy, Excitation, Fluorescence, Quenching, Excitation, Liquids, Reprints, *Benzene, *Cation electron interactions, *Electron scavenger.

In the photoionization of liquid benzene, the fluorescence yield and the fluorescence quenching by CHCl_3 increase slowly from 1900 Å to 1750 Å, rapidly from 1750 to 1400 Å, and level off from 1400 to 1150 Å. Below 1750 Å, the relative quenching constants of CHCl_3 , CCl_3Cl , and $\text{C}_2\text{H}_5\text{Cl}$ are the same as their relative reactivities with quasi-free electrons. The quenching constants extrapolate to zero at 7.1 eV, the estimated ionization potential of liquid benzene. The quenching results are consistent with the assumption that the benzene fluorescence in the photoionization region is generated by recombination of the electron with the benzene cation.

500,178

PB85-187300 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Organic Analytical Research Div.
Characterization of Polycyclic Aromatic Hydrocarbon Mixtures from Air Particulate Samples Using Liquid Chromatography, Gas Chromatography, and Mass Spectrometry.

Final rept.,
S. A. Wise, S. N. Chesler, L. R. Hilpert, W. E. May, and R. E. Rebbert. 1983, 15p
Pub. in Proceedings of Polynuclear Aromatic Hydrocarbons: Int. Symposium on Mechanisms, Methods and Metabolism (8th), p1413-1427 1983.

Keywords: *Aromatic polycyclic hydrocarbons, *Chemical analysis, *Particles, Standards, Gas chromatography, Mass spectroscopy, Samples, Mixtures, Air pollution, Reprints, *Standard reference materials, *Air pollution detection, Liquid chromatography.

Two Standard Reference Material (SRM) air particulate samples were analyzed for the determination of polycyclic aromatic hydrocarbons (PAH). The analytical methods included the combined use of liquid chromatography (LC), gas chromatography (GC), and mass spectrometry (MS) to characterize the major and minor PAH components in the samples. The analytical methods and results for these two samples are reported.

500,179

PB85-187318 Not available NTIS
National Bureau of Standards, Boulder, CO.
Shape and Dynamics of States Excited in Electron-Atom Collisions: A Comment on Orientation and Alignment Parameters by Consideration of Attractive and Repulsive Forces.
Final rept.,
N. Andersen, I. V. Hertel, and H. Kleinpoppen. 1984, 8p
Pub. in Jnl. of Physics B: At. Mol. Phys. 17, pL901-L908 1984.

Keywords: *Helium, *Magnetic moments, Electron scattering, Atomic energy levels, Excitation, Experimental design, Comparison, Dynamics, Reprints, *Atom electron interactions.

Several ways of parametrizing results of coherence and correlation analysis of atomic excitation in planar scattering experiments have been suggested over the years. Recently, Beyer and Kleinpoppen introduced new scattering amplitudes related to contributions from predominantly the attractive and the repulsive parts of the electron-atom potential. The authors clarify their relation to the so-called neutral amplitudes of Hermann and Hertel and pursue the ideas further for the example of 80 eV electron excitation of the He (2 singlet P)-state. They demonstrate that this way of parametrizing the data is directly related to the experimental observables, enables easy visualization of the shape and dynamics of the charge cloud of the excited electron, and clarifies comparison between theory and experiment.

500,180

PB85-187342 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Thermophysics Div.
Wetting Layers and Dispersion Forces for a Fluid in Contact with a Vertical Wall.
Final rept.,
R. F. Kayser, J. W. Schmidt, and M. R. Moldover. 18 Feb 85, 4p
NASA Order-H-27954B
Pub. in Physical Review Letters 54, n7 p707-710, 18 Feb 85.

Keywords: *Fluids, *Wetting, *Dispersion relations, *Ellipsometry, Stability, Van der Waals equation, Sulfur hexafluoride, Reprints.

When a liquid wets a vertical wall, wetting layers form on the wall high above the liquid-vapor meniscus. These layers are stabilized against gravity by dispersion forces. For SF_6 in contact with fused silica, the authors find layers between 20 and 40 nm thick in a range of temperatures below critical. Their results support the predictions of Dzyaloshinskii, Lifshitz, and Pitaevskii, in contrast to recent experiments which are much harder to reconcile with theory.

500,181

PB85-187359 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Thermophysics Div.
Interfacial Tension of Fluids Near Critical Points and Two-Scale-Factor Universality.
Final rept.,
M. R. Moldover. Feb 85, 12p
NASA Order-H-27954-B
Pub. in Physical Review A 31, n2 p1022-1033 Feb 85.

Keywords: *Interfacial tension, *Fluids, *Critical point, *Liquid phases, Thermodynamic properties, Binary mixtures(Materials), Temperature, Tables(Data), Reprints.

Data for the surface tension of pure fluids near critical points and for the interfacial tension between coexisting liquid phases of binary mixtures near consolute points are reviewed using recent theoretical values for the critical exponents and the concept of two-scale-factor universality. The observation implies that the scale factors for the critical anomaly in the free energy of these liquid-vapor systems can be estimated from measurements of the densities of the coexisting phases at all temperatures and a measurement of the capillary rise near the triple point.

500,182

PB85-187391 Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Chemical Engineering Science Div.
Thermal Conductivity of Parahydrogen.
Final rept.,
H. M. Roder. Oct 84, 5p
Pub. in Jnl. of Chemical and Engineering Data 29, n4 p382-386 Oct 84.

Keywords: *Thermal conductivity, *Hydrogen, Experimental design, Isotherms, Temperature, Density(Mass/volume), Comparison, Reprints.

The paper presents new experimental measurements of the thermal conductivity of parahydrogen for eight isotherms at temperatures from 100 to 275 K with intervals of 25 K, pressures to 12 MPa, and densities from 0 to 12 mol/L. Three additional isotherms at 150, 250, and 275 K cover para-rich compositions with para percentages varying from 86% to 73%. For these three isotherms the pressures reach 70 MPa and the density a maximum of 30 mol/L. The data for all compositions are represented by a single thermal conductivity surface in which the differences in thermal conductivity for different ortho-para compositions are accounted for in the dilute-gas term. The new measurements are compared with previous data on parahydrogen through the new correlation. It is estimated that the overall uncertainty of both experimental and correlated thermal conductivity is 1.5 percent at the 3 sigma level.

500,183

PB85-187474 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Non-Linear Behavior of Polyisobutylene Solutions as a Function of Concentration.
Final rept.,
L. J. Zapas, and J. C. Phillips. 1981, 16p
Pub. in Jnl. of Rheology 25, n4 p405-420 1981.

Keywords: *Polyisobutylene, *Nonlinear systems, Solutions, Concentration(Composition), Stress relaxation, Strain analysis, Rheological properties, Reprints, *BKZ theory.

The nonlinear behavior in simple shear of polyisobutylene (Vistanex L-100) solutions in cetane was studied for three concentrations in various shear histories. The concentrations of the solutions were 10, 15.1, and 19.3 percent by weight. It is shown that a simple superposition principle can be applied at concentrations region where the intermolecular forces are predominant for the systems and for which the potential function in the Bernstein, Kearsley and Zapas elastic fluid theory can be expressed as a product of a function of time and a function of strain. An excellent agreement was obtained with the experimental data, even for transient experiments where the shearing and normal stresses depend on time.

500,184

PB85-187490 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Thermal, Unsensitized Infrared-Laser, and Laser SiF₄ Sensitized Decomposition of 1,2-Dichloropropane.
Final rept.,
W. Tsang, J. A. Walker, and W. Braun. 1982, 5p
Pub. in Jnl. of Physical Chemistry 86, n5 p719-723 1982.

Keywords: *Decomposition reactions, *Thermal analysis, *Reaction kinetics, *Infrared spectroscopy, Chlorine organic compounds, Reprints, *Laser spectroscopy, *Propane/dichloro.

1,2 Dichloropropane decomposes via 4 reaction channels forming chloropropene-3, cis-chloropropene-1, trans-chloropropene-1 and chloropropene-2. All pathways have been observed in thermal and laser induced processes. Rate parameters for the thermal processes have been derived from comparative rate single pulse shock tube studies. The focused laser experiments, direct as well as the sensitized with SiF_4 yield product ratios which are very similar and suggest that the latter also involve a photolytic process. The cis-chloropropene-1 to trans-chloropropene-1 ratios from the laser experiments suggest that they represent a final product distribution.

500,185

PB85-187615 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Convective and Interfacial Instabilities during Solidification of Succinonitrile Containing Ethanol.
Final rept.,
R. J. Schaefer, and S. R. Coriell. 1982, 11p
Sponsored by Materials Research Society, University Park, PA. and Universities Space Research Association, Columbia, MD.
Pub. in Proceedings of Symposium on Materials Processing in the Reduced Gravity Environment of Space, Boston, Mass., November 16-18, 1981, v9 p479-489 1982.

Keywords: *Solidification, *Crystallization, *Convection, *Interfaces, Additives, Ethyl alcohol, Stability, *Succinonitrile.

Although slow convective flow is difficult to detect in solidifying metals, it can readily be observed in transparent materials by observing the motion of small neutrally buoyant particles. An excellent material for such studies is succinonitrile, which solidifies with an unfaceted solid/liquid interface and which has well characterized physical properties. For studies of solute-induced convection, ethanol is a useful addition to succinonitrile because it has a lower density and a somewhat similar molecular structure. Samples of high purity and ethanol-doped succinonitrile are solidified unidirectionally in a vertical temperature gradient. Latex microspheres, 2 micrometers in diameter, are suspended in the liquid to delineate convective flow. Convective and morphological stability are observed as a function of solute concentration and growth velocity. These measurements are compared to theoretical calculations which predict the transition from stability to instability as a function of solidification conditions. The predicted transitions occur at low concentrations and solidification velocities, so that extreme care is required to eliminate the effects of impurities or thermally-induced convection.

Field 7—CHEMISTRY

Group 7D—Physical Chemistry

500,186

PB85-187771

Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

Raman and X-Ray Investigations of Ice 7 to 36.0 GPa.

Final rept.,

G. E. Walrafen, M. Abebe, F. A. Mauer, S. Block, and G. J. Piermarini. 1982, 9p

See also AD-A116 900.

Pub. in Jnl. of Chemical Physics 77, n4 p2166-2174 1982.

Keywords: *X ray analysis, *Raman spectroscopy, *X ray diffraction, *Ice, Hydrogen bonds, Chemical bonds, Pressure, Water, Reprints, Hydroxyl radicals.

Raman spectra for ice VII to 30 GPa and x-ray lattice parameters to 36 GPa, both at room temperature, are presented and discussed. Both the Raman OH-stretching peak frequency ($\delta\nu$) and the edge distance of the body-centered cubic unit cell (a) decrease at a decreasing rate with pressure rise. This minimum suggests that a symmetric hydrogen bond, O-H-O, and thus a new structure, may result at pressures of 75 GPa, or above. An analysis of both the present and previously published data verified this relation with $A=2943/\text{cm}$ (sq A).

500,187

PB85-187789

Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

Thermodynamic Surface for Isobutane.

Final rept.,

M. Waxman, and J. Gallagher. 1982, 9p

Sponsored by American Society of Mechanical Engineers, New York.

Pub. in Proceedings of Thermophysical Properties (8th), Gaithersburg, MD, June 15-18, 1981, p88-96 1982.

Keywords: *Butanes, *Thermodynamics, *Surface chemistry, Temperature, Cryogenics, Vapor phases, Liquid phases, Ideal gases, Density(Mass/volume), Pressure, *Isobutane.

A thermodynamic surface is presented for the thermodynamic properties of isobutane for the ranges of temperature from 250 to 600 K and of pressures from 0 to 400 bar, exclusive of the critical region. The surface, expressed analytically, is in the form of the Helmholtz free energy as a function of temperature and density. The Helmholtz free energy is based upon the sum of three contributions: that of the ideal gas, of a physically based function incorporating the effects of molecular repulsion and attraction, and of a sum of residual terms that compensate for inadequacies of the physically based function. The latter two contributions are evaluated from only pressure density-temperature data. The significant deviations are in regions where exclusive of vapor pressure data, the liquid and vapor phases are not defined adequately by experimental data. The authors discuss the development of the correlation and also its possible extension to cryogenic temperatures.

500,188

PB85-187797

Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

Speciation of Arsenic in Fossil Fuels and Their Conversion Process Fluids.

Final rept.,

C. S. Weiss, E. J. Parks, and F. E. Brinckman. 1983, 18p

Pub. in Chapter in Arsenic: Ind., Biomed., Environ. Perspect., Proc. Arsenic Symposium, p309-326 1983.

Keywords: *Arsenic, *Fossil fuels, *Chemical analysis, *Environmental surveys, *Arsenic inorganic compounds, *Arsenic organic compounds, Coal gasification, Petroleum industry, Oil shale, Industrial wastes, Combustion products, Trace elements, Metals, Retorting, Water pollution, Air pollution, Reprints, *Gel permeation chromatography, Solid wastes, Coal liquefaction.

The increased use of coal and oil shale, both directly and following conversion processes, as alternatives to petroleum dictates the need to understand the chemistry and environmental fate of many toxic elements which are found at higher concentrations in these alternative fossil fuels and their processing products. These elements include As, Be, Cd, Cr, Ge, Hg and Se. The ultimate environmental availability of such elements found in these matrices will depend not only upon the molecular form originally present, but also on the chemical transformations occurring during the type

of process used to convert these materials to conventional fuels, and during their final use. The concentration and nature of one principal bioactive element, As, in the source materials (petroleum, coal, and oil shale) will be reviewed, as will the distribution of As species among products, process waters, and residues during a variety of coal conversion and oil shale retorting processes. The methods developed at NBS to speciate As in both the products and process waters generated during synthetic fuel processes rely on the chromatographic separation of the product or process water with As-selective detection. The discrete molecular speciation of As is possible in some cases. However, complexes, colloids, or macromolecular As-containing species, evident in size-exclusion chromatograms of various shale oils, must be evaluated in terms of the extent and nature of the complexing capacity of the matrix for As as well as the stability of these As-containing compounds.

500,189

PB85-187813

Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

Resolution in C-13 NMR of Organic-Solids Using High-Power Proton Decoupling and Magic-Angle Sample Spinning.

Final rept.,

D. L. Vanderhart, W. L. Earl, and A. N. Garroway.

1981, 41p

Pub. in Jnl. of Magnetic Resonance 44, n2 p361-401 1981.

Keywords: *Nuclear magnetic resonance, *Solids, *Line width, *Organic compounds, Experimental design, Carbon 13, Reprints, *Chemical shifts(Nuclear magnetic resonance).

It is found experimentally that (^{13}C) linewidths in solids are 10-100 times broader than those in liquids even though the combined techniques of high-power proton decoupling and magic angle sample spinning are employed. The combination of the latter techniques should produce spectra determined by isotropic chemical shifts just as in a liquid. Various linebroadening mechanisms are described and evaluated for semirigid, disordered (glassy) solids and ordered crystalline solids. The greater strength of secular local magnetic fields and the more restricted molecular mobility in solids versus liquids are the principal reasons for greater linewidths in solids. In particular, the importance of anisotropic bulk susceptibility is pointed out for the first time. An important perspective is that resolution will improve only marginally if at all for higher values of the static field.

500,190

PB85-187847

Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

Thermodynamic Properties for H₂O in the Ideal Gas State.

Final rept.,

H. W. Woolley. 1980, 10p

Sponsored by Verein Deutscher Ingenieure, Duesseldorf (Germany, F.R.).

Pub. in Proceedings of Int. Conference on the Properties of Steam (9th), Munich, Germany, September 10-14, 1979, p166-175 1980.

Keywords: *Thermodynamic properties, *Water, *Ideal gas, Molecular energy levels, Steam.

Ideal gas thermodynamic properties for water have been calculated recently at the National Bureau of Standards. Through the technological range of up to 1500 K, the values obtained are purely or primarily based on values for energy levels of Flaud, Camy-Peyret, and their co-workers. Energies and rotational constants for higher vibrational levels were based on data for low lying vibrational levels of H₂O essentially as fitted by Prof. W.S. Benedict of the University of Maryland, including effects of resonance.

500,191

PB85-189207

Not available NTIS

National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.

Electron-Impact Excitation of Li II: A Model Study of Wave-Function and Collisional Approximations and of Resonance Effects.

Final rept.,

R. B. Christensen, and D. W. Norcross. Jan 85, 10p

Contract DOE-EA-77-A-01-6010

Pub. in Physical Review A 31, n1 p142-151 Jan 85.

Keywords: *Lithium, *Molecular energy levels, *Mathematical models, Excitation, Ionization, Resonance,

Wave functions, Reprints, *Electron electron interactions.

Results are presented of five-state close-coupling and distorted-wave calculations for electron impact excitation of Li II from the ground state to the four $n=2$ states for energies below the ionization threshold. Sensitivity of the results to scattering approximation, target wave functions, and resonance effects is examined. The spin-allowed transitions are found to be much more sensitive to scattering approximation and to the choice of target wave functions than are the spin-forbidden transitions, but rather more strongly to the latter.

500,192

PB85-189264

Not available NTIS

National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.

Laser Studies of Near-Resonant State-Changing Collisions of Calcium 4s6s singlet S(sub 0) with the Rare Gases.

Final rept.,

M. O. Hale, and S. R. Leone. Jan 85, 10p

Grants NSF-PHY82-00805, NSF-CHE79-11340

Pub. in Physical Review A 31, n1 p103-112 Jan 85.

Keywords: *Calcium, *Rare gases, Excitation, Molecular energy levels, Reaction kinetics, Mathematical models, Resonance, Reprints, *Laser spectroscopy, *Molecule molecule interactions, Numerical solution.

State-changing collisions of Ca(4s6s singlet S(sub 0) with the rare gases are studied by pulsed laser excitation and time and wavelength-resolved detection. The total depletion rates of the 4s6s singlet S(sub 0) state with different rare gases vary by over a factor of ten, with the lighter rare gases being markedly more efficient than the heavier ones.

500,193

PB85-189272

Not available NTIS

National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.

Effects of Orbital Alignment on Inelastic Collisions of Ca(4s5p singlet P(sub 1)) with Helium.

Final rept.,

M. O. Hale, I. V. Hertel, and S. R. Leone. 10 Dec 84,

4p

Grants NSF-PHY82-00805, NSF-CHE79-11340

Pub. in Physical Review Letters 53, n24 p2296-2299, 10 Dec 84.

Keywords: *Calcium, *Helium, *Inelastic scattering, Reprints, *Molecule molecule interactions.

The relative cross section for the process Ca(4s5p singlet P(sub 1)) + He yields Ca(4s5p triplet P(sub j)) + He + $\Delta E = 177/\text{cm}$ is determined as a function of initial alignment of the Ca(4s5p singlet P(sub 1)) state. The experiment is carried out with pulsed laser excitation in a crossed beam. These results are discussed in terms of physical models of the curve-crossing interaction.

500,194

PB85-189314

Not available NTIS

National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.

Resonant Two-Photon Ionization and Dissociation of the Hydrogen Atom and Molecule.

Final rept.,

K. H. Welge, and H. Rottke. 1984, 10p

Pub. in Proceedings of Int. Conf. on Multiphoton Processes (3rd), Iraklio, Crete, Greece, September 5-12, 1984, p48-57.

Keywords: *Hydrogen, *Ionization, *Dissociation, Excitation, Stark effect, Resonance, *Hydrogen atoms.

The authors report on two experimental studies: (A) the ionization of the H atom in strong external electric fields around the ionization limit by state-selective two-photon, one-photon resonant excitation through single sublevels of the $n=2$ Stark manifold as intermediate step, and (B) the two-photon, one-photon resonant ionization and dissociation of the H₂ molecule through selected rotational-vibrational levels of the B(sup 1) sigma(+1)(sub u) electronic state as intermediate step.

500,195

PB85-189348

Not available NTIS

National Bureau of Standards (NML), Gaithersburg, MD. Inorganic Analytical Research Div.

Quality Assurance and Protocols in Sampling and Sample Preparation of Biological Samples.

Final rept.,
R. Zeisler, and S. A. Wise. 1985, 23p
Pub. in Chapter 15 in Biological Reference Materials: Availability, Uses, and Need for Validation of Nutrient Measurement, p257-279 1985.

Keywords: *Samples, *Trace elements, *Quality assurance, *Environmental surveys, *Chemical analysis, Sampling, Concentration(Composition), Liver, Storage, Laboratories, Reprints, *Biological processes.

The apparent concentrations of trace constituents in biological samples, as opposed to the true concentrations, can be critically influenced by sampling steps prior to analysis. A multilevel approach is required to preserve a valid subsample for subsequent analysis, which is representative of the original bulk materials. In the NBS/EPA pilot program for environmental specimen banking, sampling protocols, sample preservation techniques and subsampling procedures have been developed and evaluated. A sampling protocol for human livers based on the above considerations is presented as the core of the pre-analysis quality assurance plan. This protocol includes step-by-step instructions for sampling the liver specimens and it can easily be modified to the use in sampling other tissues. Features of the protocol include: Use of special implements and/or techniques to minimize contamination during sample excision; shipment and storage of the samples under clean conditions at cryogenic temperatures; sample preparation in clean laboratories; and homogenization by a cryogenic homogenization technique that uses Teflon mills. The above steps provide a controlled basis for the analytical measurements which results in more accurate and intercomparable data.

500,196

PB85-189439 Not available NTIS

National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.

CO Isotopic Mixing Measurements on Nickel: Evidence for Irreversibility of CO Dissociation.

Final rept.,
D. W. Goodman, and J. T. Yates. 1983, 6p
Sponsored by Department of Energy, Washington, DC. Pub. in Jnl. of Catalysis 82, p255-260 1983.

Keywords: *Carbon monoxide, *Isotopic labeling, *Catalysis, Nickel, Dissociation reactions, Methanation, Methane, Water, Chemisorption, Reaction kinetics, Reprints.

The isotopic mixing reaction, (12 sup)C (18 sup)O + (13 sup)C (16 sup)O yields (12 sup)C (16 sup)O + (13 sup)C (18 sup)O, and the methanation reaction (3H₂ + CO yields CH₄ + H₂O) have been studied at 2 Torr CO pressure over a Ni(100) single crystal between 300 and 700 K. At 600 K the rate of the exchange reaction is a factor of 50 slower than CO hydrogenation indicating irreversibility of the CO dissociation reaction step. The steady state reaction becomes significant at approximately 850 K at which temperature a graphite layer begins to decompose, opening up free Ni sites. Various models to explain these observations are discussed.

500,197

PB85-189488 Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

Element by Element Review of their Atomic Weights.

Final rept.,
H. S. Peiser, N. E. Holden, P. De Bièvre, I. L. Barnes, and R. Hagemann. 1984, 74p
Sponsored by International Union of Pure and Applied Chemistry, Oxford (England).
Pub. in Pure and Applied Chemistry 56, n6 p695-768 1984.

Keywords: *Atomic weights, *Elements, Experimental design, Reprints, Natural emissions.

The IUPAC 'standard' atomic weights of the terrestrial occurring chemical elements are individually reviewed tracing changes during the past 25 years. Emphasized is the relevant published scientific evidence which in each case constitutes the basis for the expert judgment by the responsible IUPAC Commission. It biennially reports on, recommends, and tabulates the best values of these atomic weights with an implied judgement of their individual reliability. In the introductory

part of this Review the history of atomic-weight determinations is sketched. The IUPAC leadership in this data-evaluation project is described as it benefits science, technology, and trade. The remaining experimental uncertainties and natural variabilities are discussed. The treatment of abnormal materials is explained. The principal techniques for determining atomic weights are outlined. The effects of naturally occurring radioactive nuclides are characterized in their essentials.

500,198

PB85-189504

Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Organic Analytical Research Div.

Synthesis and Characterization of C18 Stationary Phases for the Liquid Chromatographic Separation of Polycyclic Aromatic Hydrocarbons.

Final rept.,
L. C. Sander, and S. A. Wise. 1983, 12p
Pub. in Proceedings of Polynuclear Aromatic Hydrocarbons: Int. Symposium on Mechanisms, Methods, and Metabolism (8th), p1133-1144 1983.

Keywords: *Aromatic polycyclic hydrocarbons, *Synthesis(Chemistry), Separation, Substrates, Comparison, Polymers, Mixtures, *Reverse phase liquid chromatography, Monomers.

A number of monomeric and polymeric C18 bonded phases were synthesized on a variety of silica substrates to evaluate selectivity differences for the liquid chromatographic (LC) separation of polycyclic aromatic hydrocarbons (PAH). The results of this study indicate which parameters (i.e., phase type, surface coverage, and silica pore diameter) are responsible for providing optimum selectivity for the separation of PAH. Comparisons of phase types indicated that polymeric C18 phases on wide pore silica substrates (300 Å) were most effective in separation of a sixteen-component PAH mixture. A simple empirical LC test was devised to gauge the extent of the monomeric or polymeric nature of a phase.

500,199

PB85-189512

Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Thermophysics Div.

Simulation of the Initiation of Detonation in an Energetic Molecular Crystal.

Final rept.,
D. H. Tsai, and S. F. Trevino. 15 Dec 84, 2p
Pub. in Jnl. of Chemical Physics 81, n12, pt. 1, p5636-5637, 15 Dec 84.

Keywords: *Detonation, *Mathematical models, *Exothermic reactions, Dissociation reactions, Chemical reactions, Shock waves, Reprints, *Molecular crystals.

A molecular dynamical study of the detonation process in a dense system is presented. The model is a filament of a molecular crystal capable of undergoing exothermic dissociation. When the model is heated at one end, dissociation reactions start at the heated end and propagate along the filament. The accompanying expansion of the heated region drives a shock wave into the filament, causing further reactions due to shock heating. The results thus obtained provide a molecular description of the initiation of detonation.

500,200

PB85-189520

Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Molecular Spectroscopy Div.

Compact Effective Potentials and Efficient Shared-Exponent Basis Sets for the First- and Second-Row Atoms.

Final rept.,
W. J. Stevens, H. Basch, and M. Krauss. 15 Dec 84, 8p
Pub. in Jnl. of Chemical Physics 81, n12, pt. 2, p6026-6033, 15 Dec 84.

Keywords: *Atoms, *Potential theory, Atomic energy levels, Normal density functions, Reprints, *Effective-range theory, *Pseudopotential theory, Pseudospectral methods, Numerical solution, Gaussian measures.

Compact effective potentials, which replace the atomic core electrons in molecular calculations, are presented for atoms in the first and second rows of the periodic table. The angular-dependent components of these potentials are represented by compact one- and two-term gaussian expansions obtained directly from the appropriate eigenvalue equation. Energy-optimized gaussian basis set expansions of the atomic

pseudo-orbitals are also presented. The basis sets consist of four gaussian functions which have a common set of exponents (shared-exponents) for the s and p orbitals. The potentials and basis sets have been used to calculate the equilibrium structures and spectroscopic properties of several molecules. The results compare extremely favorably with corresponding all-electron calculations.

500,201

PB85-191427

PC A03/MF A01
National Physical Lab., Teddington (England). Div. of Material Applications.

Coordinated Development of Standards for Surface Chemical Analysis.

M. P. Seah, and C. J. Powell. Mar 85, 41p NBSIR-85/3120

Keywords: *Surface chemistry, *Standards, *Chemical analysis, Coatings, Films, *Standard reference materials, Versailles project.

This report is based on a proposal to the Steering Committee of the Versailles Project on Advanced Materials and Standards (VAMAS) for the coordinated development amongst the VAMAS member states of standards for surface chemical analysis. VAMAS was established following a meeting of the Heads of State or government at Versailles, France in 1982 that agreed on a number of projects relating to technology, growth, and employment. Specifically, VAMAS was organized to promote international coordination in the development of standards in a wide range of advanced material sectors. Surface chemical analysis was approved as a VAMAS Technical Working Area in June, 1984. The report describes the growth and diversity of surface analysis in the development of advanced materials in modern technologies and additionally, the use of surface analysis for improved films and coatings. The principal techniques of surface analysis in common use are identified and the technical limitations to accurate surface analyses identified. Specific needs are identified for the common methods of surface analysis, Auger-electron spectroscopy, x-ray photoelectron spectroscopy, and secondary-ion mass spectroscopy together with the needs for ion sputtering which is used to obtain composition versus depth information in films and coatings. Existing standards activities in the member countries of VAMAS are reviewed and suggestions are made for additional standards for surface chemical analysis.

500,202

PB85-195907

Not available NTIS
National Bureau of Standards, Gaithersburg, MD.

Infrared Laser-Induced Decomposition of Diethyl Ketone and n-Butane.

Final rept.,
M. J. Pilling, J. R. McNesby, and W. Braun. 1981, 15p
Sponsored by Maryland Univ., College Park.
Pub. in Jnl. of Photochemistry 17, n3-4 p281-295 1981.

Keywords: *Decomposition reactions, *Mathematical models, Infrared lasers, Reprints, *Laser induced reactions, *Ketone/diethyl, *Butane, Laser applications.

The focused, IR Laser-induced decomposition of diethyl ketone has been studied and compared with the SiF₄-sensitized decomposition of diethyl ketone and n-butane. A model has been constructed for the direct decomposition of diethyl ketone involving total decomposition of diethyl ketone into ethyl radicals and CO near the focus. Reaction between ethyl radicals form a short-lived n-butane which decomposes statistically into two ethyls or two methyls and ethylene. The system is allowed to react with due account being taken of unimolecular fall-off behavior for all species. The temperature which best explains the experimental product distribution is 1400 K. SiF₄-sensitized decomposition of diethyl ketone and n-butane appear to be characterized by purely thermal processes.

500,203

PB85-195998

Not available NTIS
National Bureau of Standards, Gaithersburg, MD.

Equation of State Theories of Polymer Blends.

Final rept.,
I. C. Sanchez, and K. Solc. 1982, 18p
Pub. in Polymer Compatibility and Incompatibility, Principles and Practices, Midland Macromolecular Meeting (10th), p59-76 1982.

Field 7—CHEMISTRY

Group 7D—Physical Chemistry

Keywords: *Polymers, *Equations of state, *Phase diagrams, Blends, Mixtures, Stability, Critical temperature, Thermodynamics, Entropy.

Phase diagrams of liquid polymer/polymer mixtures (blends) are very unusual when compared to similar low molecular weight mixtures. Neither the familiar adage 'likes dissolve likes' nor the familiar observation that solubility increases with temperature are in general applicable to polymer blends. In this paper, the authors examine the thermodynamic and molecular reasons responsible for this unusual phase behavior. A general thermodynamic analysis of phase stability is presented which suggests that thermally induced phase separation near a low critical solution temperature is an entropy driven process. The entropic driving force is related to the compressible nature of a fluid mixture and the propensity of fluids to contract upon mixing (negative volume changes) at sufficiently high temperatures, or equivalently, sufficiently low fluid densities. By using molecular equation of state theories, they are able to show that volume contraction is always expected at low fluid densities if attractive interactions exist between dissimilar molecular species. All of the unusual aspects of polymer blend phase behavior can be given a rational basis.

500,204
PB85-196046 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Development and Use of Numeric Physical/Chemical Properties Databases.
Final rept.,
S. P. Fivozinsky. 1982, 12p
Pub. in Drexel Library Quarterly 18, n3/4 p27-38 1982.

Keywords: *Physical properties, *Chemical properties, *Information systems, Utilization, Forecasting, Reprints.

This article presents a glimpse of activities which are producing and disseminating numeric physical and chemical databases. The discussion defines evaluated databases, looks at the history and present organization of major U.S. activities, examines the structure of similar programs in other countries, and projects into the future.

500,205
PB85-196061 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Lifetime Prediction from Polymer Degradation Kinetics.
Final rept.,
J. H. Flynn. 1982, 1p
Pub. in Proceedings of the International Symposium on I.U.P.A.C., Macromolecules, 1982, p322.

Keywords: *Reaction kinetics, *Degradation, *Life(Durability), *Life tests, *Thermogravimetry, Materials tests, Polyurethane resins, Polyester resins, Polyether resins, Diisocyanates, Polymers, Isocyanic acid/methylene-(diphenylene-ester)-di, Isocyanic acid/(methylphenylene-ester).

New techniques for measuring kinetics parameters at low conversion and over a wide range of heating rates were applied to thermogravimetric data on MDI and TDI, polyether and polyester soft segment, polyurethanes. Use of higher molecular weight diisocyanates and surface blockage are suggested as means to obtain improved durability.

500,206
PB85-196079 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Effect of Striations on the Compositional Analysis of Silicon Crystals.
Final rept.,
R. A. Forman, M. I. Bell, A. Baghdadi, and S. Mayo. 1983, 10p
Sponsored by Electrochemical Society, Inc., Pennington, NJ, Electronics Div.
Pub. in Proceedings of Symposium on Defects in Silicon, San Francisco, CA., May 8-13, 1983, the Electrochemical Society, v83 n9 p303-312.

Keywords: *Silicon, *Chemical analysis, Composition(Property), Crystal growth, Periodic variations, Striations, Impurities, Carbon, Oxygen, Crystal defects, Semiconductors, Gettering.

Periodic variations of composition along the growth direction in semiconductor crystals commonly arise from fluctuations in the local growth rate. These striations of impurity content can lead to systematic errors in com-

positional analysis by optical transmission or surface analysis techniques. A model appropriate for the analysis of such measurements is presented, and estimates of probable errors are given. The model is applied to earlier published measurements on the carbon and oxygen content of silicon. The implications of these results for studies of intrinsic gettering are discussed.

500,207
PB85-196087 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Photoacoustic Detection of HCl.
Final rept.,
A. Fried, and W. Berg. 1983, 3p
Pub. in Optics Letters 8, n3 p160-162 Mar 83.

Keywords: *Trace elements, *Hydrogen chloride, Performance evaluation, Laboratory equipment, Reprints, *Atmospheric chemistry, *Photoacoustic effect.

A sensitive photoacoustic detection system for trace atmospheric measurements of HCl is described. The results reported here suggest the capability of measuring HCl at the 50 ppb level with a prototype laboratory system. Further system improvements and atmospheric measurements considerations are discussed.

500,208
PB85-196152 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Studies of Liquid Metal Surfaces Using Auger Spectroscopy.
Final rept.,
S. C. Hardy, and J. Fine. 1982, 9p
Sponsored by Universities Space Research Association, Columbia, MD., and Materials Research Society, University Park, PA.
Pub. in Proceedings of Materials Research Society Annual Meeting: Materials Processing in the Reduced Gravity Environment of Space, Boston, MA., November 16-18, 1981, v9 p503-511 1982.

Keywords: *Surface chemistry, *Liquid metals, Concentration(Composition), Adsorption, Surface tension, Chemical composition, Temperature, *Gallium tin alloys, *Auger spectroscopy.

The surface composition of liquid gallium-tin alloys has been studied in an Auger electron spectrometer (AES) as a function of bulk composition and temperature. The sessile drop samples were cleaned by argon ion bombardment sputtering of the liquid. This technique produced surfaces that were entirely free of impurities within the sensitivity of AES and remained so for many days. Tin was found to be strongly adsorbed at the liquid-vacuum interface. The surface concentrations measured by AES are in reasonably good agreement with values calculated from surface tension measurements assuming a monolayer distribution for the adsorbed tin.

500,209
PB85-196202 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Infrared Photoluminescence in Polyacetylene.
Final rept.,
E. A. Imhoff, D. V. Fitchen, and R. E. Stahlbush. 1982, 4p
Pub. in Solid State Communications 44, n3 p329-332 Oct 82.

Keywords: *Photoluminescence, *Infrared spectroscopy, Sampling, Semiconductors, Reprints, *Polyacetylene.

More extensive photoluminescence measurements of polyacetylene reveal a broad new emission band between 1.2 and 1.6 eV in samples with various isomeric contents. The peak energy and the intensity of this low energy luminescence decrease as the cis fraction decreases, but the band is still present in fully converted trans samples. These characteristics suggest that the infrared emission either is due to perturbed fragments of cis polyacetylene or is unquenched (sup 1)Ag luminescence from segments of trans (CH)_x.

500,210
PB85-196210 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Early Hydration of Large Single Crystals of Tricalcium Silicate.
Final rept.,
J. B. Ings, P. W. Brown, and G. Frohnsdorff. 1983, 6p
Pub. in Cement and Concrete Research 13, n6 p843-848 Nov 83.

Keywords: *Calcium silicates, *Hydration, *Crystals, *Surface chemistry, Calcium hydroxide, Cements, Concrete products, Construction materials, Reprints.

A reaction product believed to be an initial hydrate layer was observed to have formed on large pure C3S single crystals after 5 minutes of hydration. This layer was then increased in thickness and became covered with micrometer-sized spheres of poorly crystallized Ca(OH)₂, within 30 minutes. Subsequently, the formation of a new hydration of acicular morphology was observed to occur on the surface of the first-formed hydrate. This transformation was accompanied by the disappearance of the first hydrate layer and the calcium hydroxide spheres.

500,211
PB85-196244 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Emission and Predissociation of Li2(+1) (sup 2)Pi(sub u).
Final rept.,
P. S. Julienne. 1982, 4p
Pub. in Chemical Physics Letters 87, n3 p240-243, 26 Mar 82.

Keywords: *Emission spectroscopy, *Reaction kinetics, Radioactive age determination, Reprints, *Lithium ions, *Predissociation, Ab initio properties.

The spontaneous (sup 2)Pi(sub u) - (sup 2)Sigma(+1)(sub b) radiative emission rates and predissociation rates of (sup 2)Pi(sub u) by (sup 2)Sigma(+1)(sub u) are calculated for the (sub u) state of Li2(+1) using ab initio transition matrix elements. The phi branches are not predissociated, whereas the P and R branches are predissociated in a manner that varies strongly with vibrational and rotational quantum numbers. The v = 0 (sub u) radiative lifetime is 12 ns.

500,212
PB85-197424 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Reaction Products from a Microwave Discharge in N2 and H2S. 1. The Microwave Spectrum of NS.
Final rept.,
F. J. Lovas, and R. D. Suenram. 1982, 7p
Pub. in Jnl. of Molecular Spectroscopy 93, n2 p416-422 Jun 82.

Keywords: *Microwave spectra, Molecular energy levels, Interstellar matter, Radio astronomy, Molecular rotation, Reprints, *Nitrogen sulfide.

The microwave spectrum of NS has been reinvestigated in order to provide more accurate molecular constants, and measured and predicted transition frequencies for radio astronomers. The analysis follows earlier studies but provides an improvement in the accuracy of the molecular constants which is essential for predicting higher frequency transitions for radio astronomy. The calculated transitions range up to the N=6-5 levels with an accuracy on the order of 1 MHz.

500,213
PB85-197432 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Reactions of Sulfur(IV) with Transition-Metal Ions in Aqueous Solutions.
Final rept.,
R. E. Huie, and N. C. Peterson. 1983, 30p
Pub. in Advances in Environmental Science and Technology 12, p117-146 1983.

Keywords: *Sulfur, *Transition metals, *Oxidation reduction reactions, Ions, Air pollution control equipment, Scrubbers, Flue gases, Oxidation, Corrosion, Solutions, Reprints, *Acid rain, *Chemical reaction mechanisms.

The redox and complexation reactions of S(IV) with transition metal ions was reviewed, with emphasis on the mechanism of the oxidation of S(IV). Primary emphasis was on the reactions of Fe(III), Cu(II), Mn(III), and Co(III), but others, such as Hg(II), Cu(III), and Ir(IV) were also discussed. The results were analyzed and the proposed mechanisms discussed. Suggestions were given for the experimental work needed to establish the mechanism of the oxidation of S(IV) by transition metal ions.

500,214
PB85-197473 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.

Dielectric Friction and Ionic Mobility in Polar Liquids and Liquid Crystals.

Final rept.,
J. B. Hubbard, R. F. Kayser, and P. J. Stiles. 1983, 2p
Pub. in Chemical Physics Letters 95, n4-5 p399-401 1983.

Keywords: *Dielectric properties, *Liquid crystals, *Ionic mobility, *Mathematical models, Friction, Molecular relaxation, Comparison, Diffusion, Transport properties, Reprints, *Polar liquids.

The authors introduce a continuum model of dielectric friction on an ion in a polar liquid. This model couples hydrodynamic motions of the polarized solvent to dielectric relaxation by both rotational diffusion and translational diffusion of solvent molecules. They show that in solvents with sufficiently long dielectric relaxation times, translational diffusion is the dominant relaxation mechanism. They compare their predictions with experimental data on ion mobilities in nematic liquid crystals.

500,215

PB85-197515 Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

Preparation and Certification of Standard Reference Materials to Be Used in the Determination of Retained Austenite in Steels.

Final rept.,
G. E. Hicho, and E. E. Eaton. 1983, 4p
Pub. in Advances in X-Ray Analysis 26, p137-140 1983.

Keywords: *Chemical analysis, *X ray fluorescence, *Austenite, *Steel constituents, *Stainless steel, Standards, X ray analysis, X ray diffraction, Calibrating, Reprints, *Standard reference materials.

X-ray Standard Reference Materials have been prepared to aid diffractionists in their determination of retained austenite in hardened steels. Using powder metallurgical techniques, two groups of powder compacts, containing nominally 5, and 30% austenite in a matrix of ferrite, were prepared from 310 austenitic stainless steel and 430 ferritic stainless steel powders. The compacts, approximately 21 mm diameter, 3 mm thick, were subsequently ground, polished, and characterized. The significant difference in nickel contents of each component, 20 weight percent in the 310 as compared to .09 in the 430, allowed the use of X-ray fluorescence to determine the weight percent nickel on each compact's surface. Compacts were then ranked from lowest to highest nickel content and a predetermined number of samples were selected from each population in order to establish calibration curves. Each calibration curve related the weight percent nickel, as determined by X-ray fluorescence, to the area percent austenite as determined by quantitative metallographic examination of a compact's stained surface. Using the calibration curve, the area percent austenite (i.e., volume percent) was subsequently assigned to each corresponding weight percent nickel. A number of specimens were selected from each group and the volume percent austenite was determined by X-ray diffraction. Results show good agreement with the value obtained from the calibration curve for these compacts.

500,216

PB85-197564 Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

Mechanism of O3-Aldehyde Reactions.

Final rept.,
R. I. Martinez. 1982, 13p
Pub. in International Jnl. of Chemical Kinetics 14, n3 p237-249 1982.

Keywords: *Ozone, *Aldehydes, *Chemical reactions, Reprints, *Chemical reaction mechanisms.

Examination of the recent work of several investigators indicates that the currently-accepted O3-aldehyde reaction mechanism is incomplete, and an alternative mechanism is proposed to explain the observations.

500,217

PB85-197598 Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

Infrared Spectrum of Stannous Oxide (SnO).

Final rept.,
A. G. Maki, and F. J. Lovas. 1983, 8p
Pub. in Jnl. of Molecular Spectroscopy 98, n1 p146-153 Mar 83.

Keywords: *Infrared spectra, *Tin oxides, High temperature tests, Least square method, Molecular energy, Vapor phases, Isotopes, Reprints, *Laser spectroscopy.

A tunable diode laser has been used to measure the infrared spectrum of stannous oxide (SnO) in the gas phase between 830/cm and 868/cm. Measurements of the $\nu = 1-0$, 2-1, 3-2, and 4-3 transitions have been made at temperatures ranging from 930C to 1150C. Over 175 infrared transitions of the nine most abundant SnO isotopic species have been combined with microwave measurements reported by others in a single least-squares analysis of the data to yield a set of eight Dunham coefficients for the $X(\text{sup } 1)$ Sigma(sup +) state of SnO.

500,218

PB85-197614

Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

Thermodynamic Surface for the Critical Region of Ethylene.

Final rept.,
J. M. H. L. Sengers, J. S. Gallagher, F. W. Balfour, and J. V. Sengers. 1982, 9p
Sponsored by American Society of Mechanical Engineers, New York and National Science Foundation, Washington, DC. See also PB84-217850.
Pub. in Proceedings of Symposium on Thermophysical Properties (8th), Gaithersburg, MD., June 15-18, 1981, Volume 1: Thermophysical Properties of Fluids, p368-376 1982.

Keywords: *Thermodynamic properties, *Surface chemistry, *Ethylene, *Critical point, Equations of state, Scaling, Fluids, Speed of sound, Vapor pressure, Comparison, Experimental design, PVT properties.

The anomalous thermodynamic behavior of fluids near the critical point is described by a thermodynamic potential the authors introduced before. It has the following features: dependent and independent variables are intensive; the thermodynamic properties are analytic throughout the one-phase region except at the critical point; the asymptotic critical behavior is described by Ising-model critical exponents; liquid-vapor asymmetry is incorporated by means of 'mixing of variables'; one correction term to asymptotic scaling is used. A complete formulation of thermodynamic properties is presented here. For ethylene, the thirteen adjustable parameters in the potential were determined by a fit to PVT, vapor pressure and speed-of-sound data. Comparison with experimental data and with other recent formulations are presented.

500,219

PB85-197648

Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

New Representation for Thermodynamic Properties of a Fluid.

Final rept.,
F. Kohler, and L. Haar. 1981, 7p
Pub. in Jnl. of Chemical Physics 75, n1 p388-394, 1 Jul 81.

Keywords: *Fluids, *Thermodynamic properties, Equations of state, Thermodynamic properties, Density(Mass/volume), Helmholtz free energy, Reprints, Virial coefficients.

It is proposed to consider the contribution of the non-isolated molecular pairs to the configurational Helmholtz' energy, i.e., the quantity $f^*/RT B(\rho)$, where the product of second virial coefficient beta times molar density rho covers the contribution of the isolated pairs. The difference function can be correlated empirically in a simple way and can be used for estimating thermodynamic properties at intermediate and low densities from high density results.

500,220

PB85-197689

Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

Electrodynamics of an Ion Near the Surface of a Conducting Dielectric.

Final rept.,
R. F. Kayser, and J. B. Hubbard. 1982, 10p
Pub. in Jnl. of Chemical Physics 77, n9 p4704-4713, 1 Nov 82.

Keywords: *Electrodynamics, *Surfaces, *Ions, *Solids, *Dielectric properties, Conductivity, Reprints.

The authors investigate the electrodynamic phenomena associated with an ion moving near the flat surface of a conducting dielectric solid, where the

medium containing the ion has an arbitrary dielectric constant, and the solid has a surface conductivity which is independent of its bulk conductivity. For a fixed ratio of surface to bulk conductance, they show that the frictional drag on the ion is dominated by surface dissipation if the ion is sufficiently close to the surface, while bulk (i.e., ohmic) dissipation is the dominant drag mechanism at large distances. The energy dissipation turns out to be independent of the dielectric constants of the two media, given that dielectric dispersion effects are neglected.

500,221

PB85-197697

Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

Mechanism of Fischer-Tropsch Synthesis on a Single Crystal Nickel Catalyst.

Final rept.,
R. D. Kelley, and S. Semancik. 1983, 4p
Pub. in Jnl. of Catalysis 84, n1 p248-251 1983.

Keywords: *Hydrogen, *Carbon monoxide, *Catalysts, *Surface chemistry, Molecular weight, Pressure, Reprints, *Chemical reaction mechanisms, *Auger spectroscopy, Fischer-Tropsch synthesis.

Reactions of H2 and CO over a Ni(100) model catalyst have been studied. Measurements of the surface carbon concentrations and the product yields show that, for a fixed carbon level, the amounts of higher molecular weight hydrocarbons are strongly dependent on the reactant carbon monoxide pressure, and suggest a formation mechanism that involves a CO insertion step.

500,222

PB85-197713

Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

Extension of the Square-Gradient Theory to Fourth Order.

Final rept.,
R. F. Kayser, and H. J. Raveche. 1983, 9p
Pub. in Physica A 120A, n1-2 p68-76 1983.

Keywords: *Helmholtz free energy, *Fluids, Reprints, *Square gradient theory, Pair correlation function.

In the square-gradient theory, the Helmholtz free energy density of a nonuniform fluid is approximated by that of a uniform fluid plus a term proportional to the square of the density gradient. Presented here is the extension of this theory (and the corresponding theory of the chemical potential) to fourth order in the gradients. The new results can be applied to study the pair correlation function and interfacial density profile in a fluid near its critical point.

500,223

PB85-197721

Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

Ohmic Friction of an Ion in a Conducting Pore.

Final rept.,
R. F. Kayser, and J. B. Hubbard. 1983, 3p
Pub. in Jnl. of Chemical Physics 78, n4 p1935-1937, 15 Feb 83.

Keywords: *Ion currents, Energy dissipation, Reprints, Ionic conductivity.

The authors computed the energy dissipation associated with an ion moving along the axis of a cylindrical pore, the exterior of which is a conductor.

500,224

PB85-197754

Not available NTIS

National Bureau of Standards (NML), Gaithersburg, MD.

Inorganic Analytical Research Div.

Critical Review of Measurement Practices for the Determination of pH and Acidity of Atmospheric Precipitation.

Final rept.,
G. Marinenko, and W. F. Koch. 1984, 5p
Sponsored by Environmental Protection Agency, Washington, DC.
Pub. in Environment International 10, p315-319 1984.

Keywords: *Air pollution, *pH, *Acidity, *Precipitation(Meteorology), Reviews, Standards, Volumetric analysis, Reprints, *Acid rain, Atmospheric chemistry.

This review surveys current literature on the measurement of pH and acidity of atmospheric precipitation. Current practices for calibrating pH-measuring systems for atmospheric precipitation applications are re-

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viewed and possible sources of error are discussed. Determinations of acidity are grouped in accordance with the type of end-point selected for titration: color indicator, fixed pH, Gran plot, and closed loop.

500,225

PB85-197762 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Molecular Spectroscopy Div.

Group Theoretical Treatment of the Planar Internal Rotation Problem in (HF)₂

Final rept.,

J. T. Hougen, and N. Ohashi. 1985, 32p

Pub. in Jnl. of Molecular Spectroscopy 109, p134-165 1985.

Keywords: *Molecular rotation, *Hydrogen fluoride, Molecular structure, Reprints, *Dimers, *Molecular configurations.

The HF dimer is believed to exhibit an internal rotation tunneling process between two planar but nonlinear equilibrium configurations, during which tunneling the roles of the hydrogen-bonded and the free hydrogen atom are interchanged. Various details of energy level diagrams, symmetry species for operators, selection rules for spectroscopic transitions, and statistical weights are presented for the (HF)₂ tunneling problem, as well as some speculation on the general question of when point groups, permutation-inversion groups, or double groups are preferable for treating large-amplitude vibrational motion problems.

500,226

PB85-197788 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Quantum Metrology Group.

Molecular X-Ray Spectra: S-K(beta) Emission and K Absorption Spectra of SCO and CS₂

Final rept.,

R. C. C. Perera, and R. E. LaVilla. 15 Oct 84, 8p

Pub. in Jnl. of Chemical Physics 81, n8 p3375-3382, 15 Oct 84.

Keywords: *X ray spectra, *Emission spectroscopy, *Absorption spectra, Comparison, Fluorescence, Reprints, *Carbonyl sulfide, *Carbon sulfide(CS₂).

The sulfur K(beta) emission in fluorescence and K absorption of SCO and CS₂ in gas/vapor phase were measured with a double crystal spectrometer. The sulfur K(beta) emission spectra were compared with the complimentary x-ray spectral data and with the MNDO and ab initio (STO-3G) MO calculations and with previous larger basis set ab initio calculations. A comparison with the x-ray spectra from CO₂ was included for completeness. In addition the S-1s binding energy was estimated for SCO and CS₂ as 2478.7 eV and 2478.1 eV, respectively. Using the MO calculations as a guide, a tentative assignment of the prominent features in the absorption spectra was made and compared with the S-L(sub 2,3) absorption and energy loss spectra.

500,227

PB85-201515 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.

Comments on 'Scaling Theory and Enthalpy of Mixing for Binary Mixtures' (and Reply).

Final rept.,

G. Morrison, G. T. Brinke, and F. E. Karasz. 1983, 3p
Pub. in Jnl. of Chemical Physics 78, n7 p4790-4792, 1 Apr 83.

Keywords: *Binary systems(Materials), *Enthalpy, Critical point, Thermodynamics, Mixing, Reprints, *Scaling theory.

A brief geometric argument showing the connection between the excess properties of mixing for binary mixtures near a critical point and the second law of thermodynamics.

500,228

PB85-201788 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.

Hydrolysis of Dicalcium Phosphate Dihydrate in the Presence or Absence of Calcium Fluoride.

Final rept.,

M. S. Tung, L. C. Chow, and W. E. Brown. Jan 85, 4p

Sponsored by American Dental Association Health Foundation, Chicago, IL.
Pub. in Jnl. of Dental Research 64, n1 p2-5 Jan 85.

Keywords: *Hydrolysis, *Calcium phosphates, pH, Temperature, Dental materials, Reaction kinetics, Thermodynamics, Chemical reactions, Reprints, *Apatite.

Effects of temperature (25 and 37°C), pH (4.9-10.5) and CaF₂ on CaHPO₄·2H₂O (DCPD) hydrolysis were studied in a pH-stat. Octa-calcium phosphate (OCP) was the product at pH 6.2-6.8 and 25-37°C; thermodynamically stable apatitic compounds were formed at higher pH and/or higher temperature. In the presence of CaF₂, apatite was the product, its crystallinity improved, and the fluoride content increased as pH of the reaction decreased. The results demonstrate the remarkable ability of fluoride to promote the hydrolysis of an acidic calcium phosphate, DCPD, to apatite.

500,229

PB85-201853 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.

In situ Monitoring of Polymerization Reactions by Excimer Fluorescence Technique.

Final rept.,

F. W. Wang, R. E. Lowry, and W. H. Grant. 1983, 15p

Pub. in Proceedings of ACS (American Chemical Society) Division of Polymeric Materials Science and Engineering, Washington, DC., August 28-September 2, 1983, p138-142.

Keywords: *Polymerization, Excitation, Molecular energy levels, Solutions, Fluorescence, Nondestructive testing, *Excimer fluorescence method, *Bis(pyrene)propane, *Bis(pyrene)decane, *Chemical reaction mechanisms.

An excimer is formed by the association of an excited molecule with another molecule in its ground state. Such an excimer is characterized by a broad structureless fluorescence which is shifted to longer wavelengths compared to the fluorescence spectrum of the isolated molecule. Intramolecular excimer fluorescence has been observed in solutions of pyrene-labeled alkanes such as 1,3-bis-(1-pyrene)propane and 1,10-bis-(1-pyrene)decane.

500,230

PB85-201861 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Molecular Spectroscopy Div.

State Selected Velocity Measurements: NO/Ru(001) Thermal Desorption.

Final rept.,

D. S. King, and R. R. Cavanagh. 1982, 3p

See also AD-A112 210.
Pub. in Jnl. of Chemical Physics 76, n11 p5634-5636 1982.

Keywords: *Velocity measurement, *Quantum interactions, *Surface chemistry, *Molecular rotation, Molecular beams, Metals, Molecules, Fluorescence, Ultra-high vacuum, Nitrogen oxide(NO), Doppler effect, Reprints, *Laser induced fluorescence, *Thermal desorption, *Molecule molecule interactions.

Quantum state specific studies of the interactions of molecules with clean, well characterized metal surfaces are quite sparse. The authors report here the first measurement of a rotational-state specific velocity distribution for thermally desorbed molecules from a single crystal metal under ultrahigh vacuum (UHV) conditions. The experiment is based on the measurement of a molecular Doppler profile using laser Excited Fluorescence techniques.

500,231

PB85-201879 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.

Acid Precipitation: The Role of O₃-Alkene-SO₂ Systems in the Atmospheric Conversion of SO₂ to H₂SO₄ Aerosol.

Final rept.,

R. I. Martinez, and J. T. Herron. 1983, 7p

Pub. in Jnl. of Environmental Science and Health 18, n6 p739-745 1983.

Keywords: *Air pollution, *Sulfuric acid, *Aerosols, Alkenes, Ozone, Sulfur dioxide, Chemical reactions, Reprints, *Acid rain, *Atmospheric chemistry, Chemical reaction mechanism.

The atmospheric conversion of SO₂ to H₂SO₄ aerosol is discussed in the context of O₃-alkene-SO₂ reactions and a mechanism is proposed.

500,232

PB85-201887 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.

Adsorption of H₂O on Ni(111); Influence of Preadsorbed Oxygen on Azimuthal Ordering.

Final rept.,

T. E. Madey, and F. P. Netzer. 1982, 12p

Pub. in Surface Science 117, n1-3 p549-560 1982.

Keywords: *Water, *Adsorption, *Surface chemistry, Azimuth, Chemical bonds, Reprints, *Electron stimulated desorption ion angular distribution, *Temperature programmed thermal desorption.

ESDIAD (electron stimulated desorption ion angular distribution), LEED and TPD (temperature programmed thermal desorption) have been used to study the adsorption of H₂O on Ni(111), both clean and with preadsorbed oxygen. On the clean surface, a fractional H₂O monolayer adsorbed at 80 K exhibits no preferred azimuthal orientation for the H-ligands; the local bonding configurations of H₂O have a nearly random distribution.

500,233

PB85-201911 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.

Karl Fischer Titration Equation on Mass Basis.

Final rept.,

F. E. Jones. 1983, 1p

Pub. in Analytical Chemistry 55, n4 p793 1983.

Keywords: *Water, *Mass, *Volumetric analysis, *Karl Fisher reagent, Calibrating, Reprints, Numerical solution.

In a previously published paper on the application of automatic Karl Fischer titration to the determination of water, an equation used to calculate present H₂O was presented. In this equation, advantage was taken of the precision and convenience of the use of calibrated syringes for measuring volume several quantities. It is the purpose of this correspondence to present an equation in which these quantities are measured on a mass basis.

500,234

PB85-201952 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.

Anthropogenic Changes in Organic Carbon and Trace Metal Input to Lake Washington.

Final rept.,

W. R. Schell, J. R. Swanson, and L. A. Currier. 1983, 8p

Pub. in Radiocarbon 25, n2 p621-628 1983.

Keywords: *Anthropology, *Sediments, *Water pollution, *Radiocarbon dating, Lakes, Air pollution, Concentration(Composition), Fuel consumption, Industrial wastes, Fallout, Reprints, *Lake Washington, Seattle(Washington).

An example of how man's contaminants are introduced, deposited and retained in sediments giving a chronological record of events has been developed for Lake Washington, Seattle. Introduction of significant amounts of both inorganic and organic compounds into the environment have been identified as originating from fossil fuel sources-such as power plants and motor vehicles. However, many organic compounds are introduced also from contemporary biogenic materials. Through the application of the combined carbon isotope analysis technique (CCIA), the authors can distinguish between fossil and contemporary carbon source classes (using ¹⁴C), and they can identify certain sources within each of these classes (using ¹³C). In order to establish the chronology of the organic carbon pollutant input to the lake sediment, the ages of the layers have been determined using ²¹⁰Pb dating techniques. The pattern observed in the sediment thus reflects the change in the local energy consumption pattern from a predominately coal to an oil based economy. From the plutonium profile they infer that mixing occurs for three or four years before the sediment layers are compacted.

500,235

PB85-201960 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.

3D-4P Transitions in the Zinclike and Copperlike Ions YX, XI; Zr XI, XII; Nb XII, XIII; and Mo XIII, XIV. Final rept., J. F. Wyart, J. Reader, and A. Ryabtsev. 1981, 7p. Pub. in Jnl. of the Optical Society of America 71, n6 p692-698 Jun 81.

Keywords: *Atomic energy levels, Ions, Reprints, Molybdenum ions, Niobium ions, Yttrium ions, Zirconium ions.

Lines occurring as satellites on the long wavelength side of the 3d(sup 10)-3d(sup 9) 4p resonance lines of Ni-like ions have been investigated with a low inductance vacuum spark and a 10.7-m spectrograph for the elements Y, Zr, Nb, and Mo. The spectra of the Cu-like ions were interpreted by generalized least-squares fits for the sequence of four ions. Line identifications and energy levels were obtained for the 3d(sup 10) 7p configuration of the Cu-like ions Y XI - Mo XIV.

500,236
PB85-201978 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Laser Production of a Very Slow, Monoenergetic Atomic Beam. Final rept., J. V. Prodan, W. D. Phillips, and H. Metcalf. 1982, 5p. Sponsored by Office of Naval Research, Arlington, VA. Pub. in Physical Review Letters 49, n16 p1149-1153, 18 Oct 82.

Keywords: *Atomic beams, *Sodium, Laser beams, Velocity, Spectroscopy, Reprints, Laser cooling, Laser trapping, High resolution.

Using a resonant, counterpropagating laser beam, the authors have reduced the velocity of atoms in a neutral, thermal sodium beam to 40 m/s, or 4% of their initial velocity. These atoms have a kinetic energy comparable to the well depth of proposed optical traps. The 'temperature' characterizing the atoms' relative-motion was reduced to 70mK.

500,237
PB85-202026 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Dispirations, Disclinations, Dislocations, and Chain Twist in Polyethylene Crystals. Final rept., D. H. Reneker, and J. Mazur. 1983, 14p. Pub. in Polymer 24, n11 p1387-1400 1983.

Keywords: *Polyethylene, Molecular structure, Reprints, *Polymeric chains, *Molecular conformation.

It is proposed that the twist in polyethylene chains that can result from crystallization and subsequent deformation aggregates at boundaries and becomes a template for further reorganization that results in the long period observed in polyethylene fibers. The observed lower density at the boundaries requires the transport of free volume to the twist boundaries. Dispirations, disclinations, and dislocations are crystallographic defects that provide the necessary transport mechanism. Twist and bend, derived from the Eulerian angles which are computed from the sets of chain internal coordinates, relate the orientation of different segments of a chain. Twist and bend are useful for the characterization of both crystallographic defects and arbitrary conformations of polymer chains. Defects, along with folds, chain ends, and ordinary edge and screw dislocations provide a basis for interpretation of structure-property relationships in solid polyethylene.

500,238
PB85-202042 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Cell Model Theory of Polymer-Solutions. Final rept., I. C. Sanchez, and D. J. Lohse. 1981, 7p. Pub. in Macromolecules 14, n1 p131-137 1981.

Keywords: *Polymers, *Solutions, Thermodynamics, Scaling, Reprints, *Cell model, Virial coefficients, Chemical potentials, Numerical solution, Flory Huggins theory.

An incompressible, statistical thermodynamic theory of a polymer solution is formulated, which takes into account concentration in homogeneities. A generalized cell model is used as the basis for the new polymer solution theory. Closed-form, parametric equations are obtained for solvent and polymer chemical potentials which only reduce to classical (Flory-Huggins) potentials when concentration homogeneity is assumed. In a

good solvent, the calculated second virial coefficient decreases with molecular weight M (sup -1/5) dependence) in good agreement with available experimental data. In dilute solutions, chain dimensions can be analytically determined; the well-known Flory excluded volume equation is obtained. The most important parameter in the cell model is the average number of chains/cell, λ . For semi-dilute solutions ($\lambda < 1$), it is shown that several important scaling results are recovered from a simple scaling hypothesis for λ .

500,239
PB85-202620 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Adsorption of Water on Aluminum(111). Final rept., F. P. Netzer, and T. E. Madey. 1983, 8p. Pub. in Surface Science 127, n1 pL102-L109 1983.

Keywords: *Water, *Adsorption, Aluminum, Surface chemistry, Reprints, Electron stimulated desorption ion angular distributions, Low energy electron diffraction, Auger electro spectroscopy.

The adsorption of H₂O on Al(111) has been studied by ESDIAD (electron stimulated desorption ion angular distributions), LEED (low energy electron diffraction), AES (Auger electron spectroscopy) and thermal desorption in the temperature range 80-700 K. The general behavior of H₂O adsorption on clean and oxygen-precovered Al(111) (θ (sub 0) < or about monolayer) is rather similar at low temperature, but a much higher reactivity for dissociative adsorption of H₂O is noted on the oxygen-dosed surface around room temperature.

500,240
PB85-202646 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Monte Carlo Electron Trajectory Calculations of Electron Interactions in Samples with Special Geometries. Final rept., D. E. Newbury, and R. L. Myklebust. 1984, 11p. Pub. in Proceedings of Pfefferkorn Conference on Electron Beam Interactions with Solids for Microscopy, Microanalysis and Microlithography (1st), Monterey, CA., April 18-23, 1982, p153-163 1984.

Keywords: *Electron scattering, *Electron probes, Monte Carlo method, Elastic scattering, Backscattering, X ray analysis, Spatial distributions, *Electron electron interactions, *Microprobe analysis, *Monte Carlo simulation, Numerical solution, Scanning electron microscopy.

Implementing a Monte Carlo simulation for application to electron sample interactions requires use of accurate treatments of elastic and testing must be carried out to ensure that the calculation yields sensible and useful results. A suitable testing procedure includes calculation of (1) electron backscatter coefficients as a function of atomic number, including any necessary adjustment of scattering parameters (2) backscatter coefficients as a function of specimen tilt; (3) backscatter and transmission coefficients for thin foils; (4) backscattered electron energy distributions; (5) electron spatial distributions; and (6) x-rays, including x-ray depth distributions and relative and absolute yields. Adapting a Monte Carlo simulation to a particular problem involving special sample geometry requires careful consideration of the interaction of the electron with the target. When the electron trajectory crosses a boundary, the segments of the trajectory in each phase must be calculated in a logical, stepwise fashion, allowing for modification of the step lengths due to variable scattering power in phases of different composition. The particular example of a planar boundary between phases of different composition is considered.

500,241
PB85-202679 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Crystal Growth Kinetics and the Lateral Habits of Polyethylene Crystals. Final rept., E. Passaglia, and F. Khoury. 1984, 14p. Pub. in Polymer 25, n5 p631-644 1984.

Keywords: *Polyethylene, *Crystal growth, *Reaction kinetics, Polymers, Lateral stability, Surface energy, Reprints.

For polyethylene crystals the aspect ratio r of the crystal dimensions in the a and b crystallographic direc-

tions depends on temperature, undercooling, solvent, concentration, and molecular weight. At steady state growth, r can be expressed in terms of the ratio of growth rates normal to the (110) and (100) faces. Writing the growth rates in terms of the kinetic theory of crystal growth yields an expression which is used to analyze experimental results for crystallization from xylene.

500,242
PB85-202687 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Hydrocarbon Type Separation of Lubricating Base Oil in Multigram Quantity by Preparative HPLC. Final rept., P. Pei, J. Britton, and S. M. Hsu. 1983, 19p. Pub. in Jnl. of Liquid Chromatography 6, n4 p627-645 1983.

Keywords: *Lubricating oils, *Chemical analysis, *Hydrocarbons, Aromatic compounds, Reprints, High performance liquid chromatography.

A preparative HPLC method has been developed to separate lubricating base oil into its three major hydrocarbon fractions: saturates, aromatics and polars. The results are directly comparable to ASTM Method D2007, 'Hydrocarbon Type Analysis by Gradient Elution Liquid Chromatography.' The new method employs a prep HPLC unit with equal dual, radically compressed columns consisting of clay and alumina/silica gel columns. Depending on the solvent elution schemes, minor components (1 to 2% by wt.) of a base oil can be isolated in multigram quantities for further study.

500,243
PB85-202695 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Effect of Sample Dissolution Procedures on X-ray Spectrometric Analysis of Biological Materials. Final rept., P. A. Pella, H. M. Kingston, J. R. Sieber, and L. Y. Feng. 1983, 2p. Pub. in Analytical Chemistry 55, n7 p1193-1194 1983.

Keywords: *Bioassay, *X ray spectroscopy, *X ray fluorescence, Cation exchange, Liver, Trace elements, Solution, Comparison, Sampling, Separation, Chemical analysis, Reprints, *Standard reference materials.

X-ray fluorescence analysis of NBS-SRM 1577, 1577a, 1577b, Bovine liver and NBS-SRM 1575 pine needles was performed after separation and preconcentration of traces of Mn, Fe, Cu, and Zn or cation exchange resin filters. Sample dissolution techniques were modified to improve the iron recovery from 60 to 90%. Results were compared to NBS certificate values and were in agreement within 10%.

500,244
PB85-202703 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Solid-State Structures of Keto-Disaccharides as Probed by Carbon-13 Cross-Polarization, 'Magic-Angle' Spinning NMR Spectroscopy. Final rept., P. E. Pfeffer, K. B. Hicks, and W. L. Earl. 1983, 13p. Pub. in Carbohydrate Research 111, n2 p181-193 1983.

Keywords: *Isotopic labeling, *Nuclear magnetic resonance, *Saccharides, Solid state physics, Carbon 13, Crystal structure, Reprints, *Cross polarization magic angle spinning, Lactulose, Maltulose.

The 15 MHz(13)C cross-polarization magic angle spinning (CP-MAS) spectra of maltulose H₂O and anhydrous lactulose were examined at different B(sub 0) and B(sub 1) field strengths. While the lactulose spectrum was insensitive to changes in these parameters, the maltulose spectrum showed significant responses. From selective relaxation experiments, a mixture of three 'forms' (based on the ratio of the C-2' carbon resonances) of both lactulose and maltulose were shown to exist in the solid state. the (1/sup H)360 MHz DMSO-OH solution spectra of the unmutarotated disaccharides were used to establish the isomeric and anomeric composition of these crystalline solids. The chemical composition of lactulose, as determined by the (1 sup)H DMSO-OH spectrum, correlated well with the CP-MAS data, however, the spectrum of unmutarotated maltulose showed the presence of only a single beta-pyranose form anomer. Based on the ratio of the lactulose tautomers determined from the (1 sup)H

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DMSO-OH spectrum (referenced to fructose), the C-2' carbon resonances representing each anomeric form of lactulose were assigned in the CP-MAS spectrum. A 'crossover' in chemical shift positions of the anomeric resonances was observed in going from solution to solid state. Furthermore, a pronounced increase in the proportion of the furanoid anomers was noted for lactulose in the crystalline state relative to solution.

500,245
PB85-202711 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Stress Relaxation of Polyvinylidene Fluoride in Ethyl Acetate Vapor.
Final rept.,
J. C. Phillips, A. Peterline, and P. F. Waters. 1983, 7p
Pub. in Polym. Mater. Sci. Eng. 49, p555-561 1983.

Keywords: *Stress relaxation, Diffusion, Sorption, Vapor pressure, Reprints, *Vinylidene fluoride polymers, Acetic acid/(ethyl-ester).

In general, the presence of a vapor or gas in a polymer matrix enhances the stress relaxation of the polymer. The diffusion process at a given strain level may also be affected by the relaxation process. By studying diffusion and relaxation simultaneously, one obtains useful information of the concurrent processes. Polyvinylidene Fluoride in Ethyl Acetate vapor was studied at 30C for different vapor pressures at a given strain level. The results indicate that the time-dependent changes due to the sorption are reflected in the stress relaxation. These effects are also enhanced by polymer anisotropy and with the equilibrium concentration of the sorbate which is roughly proportional to the vapor pressure.

500,246
PB85-202737 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Temperature and Pressure Measurements and Standards Div.
Rotational Collisional Narrowing in the NO Fundamental Q Branch, Studied with cw Stimulated Raman Spectroscopy.
Final rept.,
W. Lempert, G. J. Rosasco, and W. S. Hurst. 15 Nov 84, 5p
Pub. in Jnl. of Chemistry Physics 81, n10 p4241-4245, 15 Nov 84.

Keywords: *Raman spectroscopy, *Nitrogen oxide(NO), *Molecular rotation, Spectral lines, Line width, Inelastic scattering, Reprints.

Self-broadened NO Q-branch spectra were obtained in the pressure region about 20-100 kPa. The authors determined J-and omega-dependent pressure broadening coefficients. The observed collisional narrowing was fitted by means of a relaxation matrix theory, incorporating recent experimental and theoretical values of NO state-to-state rates. A 'fitting law' representation of the state-to-state rates yielded good agreement with both the measured broadening coefficients and the observed spectrum.

500,247
PB85-202752 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Chemical Kinetics Div.
Kinetic Isotope Effect in the Thermal Dehydration of Cellobiose.
Final rept.,
M. D. Scheer. 1985, 6p
Pub. in Fundamentals of Thermochemical Biomass Conversion, p89-94 1985.

Keywords: *Dehydration, *Reaction kinetics, *Isotope effect, *Cellobiose, Water, Deuterium compounds, Hydrogen, Reprints.

The rates of dehydration of cellobiose, with 50% deuteration of its hydroxyl hydrogens, were measured in the 190-250 C temperature range. These rates were found to be smaller and the liquefaction temperature about two degrees higher than was the case for ordinary cellobiose. This is shown to be quantitatively consistent with the previously proposed view that the process of 'melting with decomposition' is an aqueous dissolution of the sugar and its decomposition products in the eliminated water. It is also shown that the rates of elimination of D₂O relative to H₂O and HDO cannot be accounted for by consideration of the difference in zero point energies. It is concluded that there is a significant quantum mechanical tunnelling contribution to the rates of saccharide dehydration at the relatively low temperatures of these experiments.

500,248
PB85-202836 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.
Fluorescence Measurements of Diffusion in Polymer Systems.
Final rept.,
F. W. Wang, R. E. Lowry, and E. S. Wu. 1984, 18p
Pub. in Proceedings of Transport Phenomena: Migration of Gases, Liquids, and Solids in Elastomers, Denver, CO., October 24, 1984, 18p.

Keywords: *Fluorescence, *Diffusion coefficient, *Polymers, Extraction, Antioxidants, Nitrogen organic compounds, *Phenylene diamine/N-N-diphenyl, *Thiophene/di(butyl-benzoxazoly).

The diffusion coefficients for two antioxidants N, N'-diphenyl-p-phenylene-diamine (DPPD) and 2,5-di(5-tert-butyl-2-benzoxazoly)thiophene (Uvitex OB) have been measured by extraction from a low density polyethylene film into 1-propanol at 22C. Extraction was done in a special cuvet-equipped vessel which excludes oxygen during extraction and permits direct fluorescence monitoring of the extraction solvent. Oxygen exclusion eliminates errors due to fluorescence quenching and antioxidant oxidation and allows precise measurement of the diffusion coefficient. The self-diffusion coefficient of a polystyrene polymer in diethyl phthalate was measured as a function of polymer concentration. The concentration dependence of the self-diffusion coefficient was found to agree with the predictions of the scaling concepts.

500,249
PB85-202844 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Structurally Complex Organic Ions: Thermochemistry and Noncovalent Interactions.
Final rept.,
M. Mautner. 1984, 8p
Pub. in Accounts of Chemical Research 17, n5 p186-193 1984.

Keywords: *Molecular structure, *Complex ions, Hydrogen bonds, Van der Waals equation, Thermochemistry, Steric hindrance, Reprints.

The thermochemical properties of protonated organic ions B:H(+1) and of clusters or monosolvated species B1H(+1):B2 and BH(+1):H₂O are significantly affected by the following structural factors: (1) Intramolecular hydrogen bonding; (2) Multiple hydrogen bonding; (3) Steric hindrance; (4) Charge resonance and charge delocalization; (5) Attractive van-der-Waals dispersion forces.

500,250
PB85-202869 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Uniformly Valid Asymptotic Solutions of Chemical Rate Equations for Irradiation-Produced Point Defects.
Final rept.,
R. E. Mickens. 1983, 9p
Pub. in Acta Physica Polonica A 64, n1 p59-67 Jul 83.

Keywords: *Reaction kinetics, *Mathematical models, *Asymptotic series, *Point defects, Irradiation, Reprints, Numerical solution.

The authors present a perturbation technique for obtaining solutions to a pair of nonlinear coupled differential equations which model the behavior of the kinetics of irradiation-produced interstitials and vacancies. The procedure eliminates secular terms at each stage of the calculation; consequently, the solutions are uniformly valid for $0 < \tau \leq \infty$.

500,251
PB85-202877 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Comparative Rate Single Pulse Shock Tube Studies on the Thermal Stability of Polyatomic Molecules.
Final rept.,
W. Tsang. 1981, 71p
Pub. in Shock Tubes and Chemistry, p59-129 1981.

Keywords: *Thermal stability, *Polyatomic molecules, *Shock tubes, *Chemical bonds, *Bonding strength, Heats of formation, Decomposition, Polymers, Reprints.

The comparative rate single pulse shock tube technique is shown to offer unique advantages for the de-

termination of unimolecular rate parameters for the transformations of polyatomic organic molecules. The results derived from this method on bond fissions, complex fissions and isomerizations are summarized. Particularly noteworthy are the regularities and interrelationships in the rate parameters. Results on the bond fission reactions have led to rates that are much lower than originally expected. This is brought about by smaller A-factor (for the alkanes) and higher carbon-carbon bond energies. The former is suggestive of a transition state that grows 'tighter' with temperature, while the latter calls into question heats of formation of organic radicals determined by metathesis reactions. It is demonstrated that the new bond energies provide a much sounder basis for the biradical mechanism for cis-trans isomerization and small ring decyclization. Directions for future work are indicated.

500,252
PB85-202893 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Temperature and Pressure Measurements and Standards Div.
Dynamic Behaviour of the Pople and Karasz Model.
Final rept.,
P. H. E. Meijer, and M. Keskin. 1984, 8p
Contract N00014-78-C-0518, Grant NATO-1928
Pub. in Jnl. of Physics and Chemistry of Solids 45, n8-9 p955-962 1984.

Keywords: *Crystallization, *Plastics, *Dynamics, *Mathematical models, Reprints, *Pople karasz model, *Most probable path method.

Using the Pople and Karasz model for the solidification of plastic crystals, the authors construct two different sets of dynamic equations for the translational and rotational order parameters. The first is straight generalization of the Pople and Karasz model, whereby one coupling parameter is a function of the other, and vice versa. The second generalization is based on the most probable path method of Kikuchi. In order to accomplish this they start with an appropriate transformation of the parameters. It is then shown that it is necessary to incorporate the special-angular correlation in order to apply this method. Computations for both systems of equations are given to demonstrate the behavior of the long range order parameter if it is initially far from equilibrium.

500,253
PB85-203412 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.
Transduction Phenomena in Ferroelectric Polymers and Their Role in Pressure Transducers.
Final rept.,
A. S. DeReggi. 1983, 6p
Sponsored by Army Research Office, Arlington, VA, and Office of Naval Research, Arlington, VA.
Pub. in Ferroelectrics 50, p21-26 1983.

Keywords: *Transducers, *Piezoelectricity, *Pyroelectricity, *Ferroelectric materials, *Polymers, Adiabatic conditions, Heat transfer, Reprints, *Vinylidene fluoride polymers.

The facts (1) that the piezo and pyroelectricity of polyvinylidene fluoride (PVF₂) is largely secondary and (2) that polymers in general have large thermal expansion coefficients, are responsible for transduction properties where piezo and pyroelectric effects may have to be considered together. In particular, in a PVF₂ transducer subjected to compression, the adiabatic compressional heating of the polymer is calculated to give a pyroelectric response amounting to approximately -10 percent of the isothermal piezoelectric response to the same compression. The thermal time constant governing the heat exchange between the polymer and its surrounding thus is an important design parameter. This time constant sets a crossover frequency between adiabatic and non-adiabatic response.

500,254
PB85-203420 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.

Electronic Emission Spectrum of Triatomic Hydrogen. 4. Visible Bands Near 5800 Å and Infrared Bands Near 3950/cm.

Final rept.,
G. Herzberg, J. T. Hougen, and J. K. G. Watson.
1982, 24p
Pub. in Canadian Jnl. of Physics 60, n9 p1261-1284
Sep 82.

Keywords: *Emission spectra, *Tritium, *Visible spectroscopy, *Infrared spectroscopy, *Electronic spectra, Hydrogen isotopes, Reprints.

No abstract available.

500,255
PB85-203461 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.

Model of the Kinetics of High Temperature Free Radical Reactions.

Final rept.,
N. C. Peterson, T. Ishii, and W. Braun. 1981, 9p
Sponsored by Polytechnic Inst. of New York, Brooklyn.
Pub. in NATO Adv. Study Inst. Ser., Ser. C 71, p531-539 1981.

Keywords: *Reaction kinetics, *Mathematical models, *High temperature tests, Acetone, Dissociation, Infrared spectroscopy, Chemical reactions, Thermal conductivity, Reprints, *Methyl radicals.

Methyl radicals are generated by multiple photon dissociation of acetone in a small volume. The temperature rises rapidly to 2000 K and high temperature reactions take place. Rapid expansion quenches the high temperature reactions in time of the order of .00001 s. Quenching of the chemical reactions occurs rapidly by expansion and more slowly by thermal conductivity. A picture of the hydrodynamic flow, equilibration of vibrational and translational temperatures and thermal conductivity for a computer model consistent with experimental data is described.

500,256
PB85-203495 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.

Innovations in Atomic Absorption Spectrometry with Electrothermal Atomization for Determining Lead in Foods.

Final rept.,
T. C. Rains, T. A. Rush, and T. A. Butler. 1982, 5p
Pub. in Jnl. of the Association of Official Analytical Chemists 65, n4 p994-998 1982.

Keywords: *Food analysis, *Lead(Metal), Chemical analysis, performance evaluation, Comparison, Reprints, *Atomic absorption spectroscopy, *Electrothermal atomization, Standard reference materials.

A simple and rapid method is described for the determination of lead in foods. The samples are digested in HNO₃, HF, and HClO₄ and then the lead is determined by atomic absorption spectrometry using an electrothermal atomizer with the L'vov platform. Interferences and ways to improve the precision and accuracy of the analysis were studied. Matrix modification using 1 percent ammonium phosphate was found to alleviate most interferences encountered. The precision and accuracy of the method was evaluated using NBS-SRM 1570 Spinach and SRM 1566 Oyster Tissue. The values obtained are in good agreement with the certified values.

500,257
PB85-203529 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Center for Basic Standards.

Determination of the 1s Lamb Shift in One-Electron Argon Recoil Ions.

Final rept.,
H. F. Beyer, R. D. Deslattes, F. Folkmann, and R. E. LaVilla. 1985, 9p
Pub. in Jnl. of Physics B: Atomic and Molecular Physics 18, p207-215 1985.

Keywords: *Radioactive decay, *Electron spectroscopy, Atomic energy levels, Ions, Field theory, Reprints, *Argon ions, *Lamb shift, *Recoil spectroscopy.

The authors report accurate measurements of doublet P(sub 3/2, 1/2) yields 1s (Lyman-alpha(sub 1,2)) transitions in Ar(+17) produced by encounters with a U(+66) beam at 5.9 MeV/nucleon. The 'recoil' production mechanism eliminates the need for Doppler corrections while a wavelength accuracy of 5 ppm relative to visible standards is attained through use of a

transfer standard x-ray profile. This permits a 1.5% test of the 1s(sub 1/2) Lamb shift as limited by model uncertainties arising from spectator electron satellites.

500,258
PB85-205185 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.

Measurement of the 1s Lamb Shift in Hydrogenlike Chlorine.

Final rept.,
P. Richard, M. Stockli, R. D. Deslattes, P. Cowan, and R. E. LaVilla. May 84, 4p
Sponsored by Department of Energy, Washington, DC.
Pub. in Physical Review A 29, n5 p2939-2942 May 84.

Keywords: *Atomic energy levels, *X ray analysis, Excitation, Fine structure, Reprints, *Lamb shift, *Beam foil excitation, *Chlorine ions.

The 1s Lamb shift in hydrogenlike chlorine has been determined from a precision measurement of x-ray transitions using beam-foil excitation. The x-rays are emitted from high-velocity chlorine-ion beams at several ion velocities produced by a Van de Graaf accelerator. The 1s Lamb shifts obtained from the Ly(alpha 1) + Ly(alpha 2) measurements are 0.84(12) and 0.90(10) eV, respectively, compared with a calculated value of 0.9384(6) eV. The fine-structure splitting of the 2p level was also determined in the experiment and found to be 3.889(30) eV compared with a theoretical value of 3.82718(2) eV. A precision measurement of the Ar K alpha x rays was made in order to establish the energy scale for Cl Ly(alpha) x-rays.

500,259
PB85-205193 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.

Estimated Thermodynamic Functions for Some Chlorinated Benzenes, Phenols, and Dioxins.

Final rept.,
W. M. Shaub. 1982, 34p
Pub. in Thermochimica Acta 58, n1 p11-44 1982.

Keywords: *Thermodynamics, *Benzenes, *Phenols, *Dioxins, *Chlorine organic compounds, Molecular structures, Molecular vibration, Reprints, Dibenzodioxins, Polychlorinated biphenyls, Chlorinated dibenzodioxins.

Procedures for estimating the values of gas phase thermodynamic functions for a large number of chlorinated benzenes, phenols and dioxins (dibenzo-p-dioxins) have been developed from estimated values of molecular parameters. Structurally similar model compounds were used to make frequency assignments, and when available, interatomic distances were taken from the literature. Symmetry numbers were assigned based upon known structures.

500,260
PB85-205201 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.

Preparation of Gas Cylinder Standards for the Measurement of Trace Levels of Benzene and Tetrachloroethylene.

Final rept.,
W. P. Schmidt, and H. L. Rook. 1983, 5p
Pub. in Analytical Chemistry 55, n2 p290-294 1983.

Keywords: *Trace elements, *Gas cylinders, *Standards, *Gravimetric analysis, *Chemical analysis, Performance evaluation, Mixtures, Reprints, *Benzene, *Ethylene/tetrachloro.

A procedure to prepare primary gas cylinder standards for benzene and tetrachloroethylene at trace levels (0.2-10 ppm) was developed. Gas mixtures prepared by this procedure were intercompared using GC-FID over a period of one year and were determined to be stable and accurate. Mixtures of these organics in nitrogen were generated dynamically using gravimetrically-calibrated permeation tubes and these mixtures were compared with the gas cylinder standards to further confirm the accuracy of the preparative technique.

500,261
PB85-205268 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Electrosystems Div.

Observation of Prebreakdown and Breakdown Phenomena in Liquid Hydrocarbons Under Nonuniform Field Conditions.

Final rept.,
R. E. Hebner, E. F. Kelley, E. O. Forster, and G. J. FitzPatrick. Jul 84, 5p
See also PB83-135160.

Pub. in Proceedings of Int. Conf. on Conduction and Breakdown in Dielectric Liquids (8th), Pavia, Italy, July 24-27, 1984, IEEE (Institute of Electrical and Electronics Engineers) Conf. Record No. 84CH2055-2, p185-189.

Keywords: *Electrical faults, *Electrical discharges, Electrical insulators, Field tests, Dielectric properties, Hexane, Toluene, Impurities, Cathode, Anode, Ionization potentials, Insulating oil, Marcol 70.

The prebreakdown processes have been recorded in n-hexane, toluene, and Marcol 70, both in a pure state and with selected impurities. The study was carried out using a point-plane geometry. A low ionization potential additive had only a small effect on the breakdown voltage or the streamer propagation speed but did significantly alter the shape of the prebreakdown streamer when the needle was the anode. For a cathode needle, chemical impurities affected the breakdown voltage.

500,262
PB85-205292 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.

Transduction Phenomena in Ferroelectric Polymers and Their Role in Biomedical Applications.

Final rept.,
A. S. DeReggi. 1984, 23p
Sponsored by Army Research Office, Arlington, VA. and Office of Naval Research, Arlington, VA.
Pub. in Ferroelectrics 60, p83-105 1984.

Keywords: *Ferroelectric materials, *Polymers, *Transducers, *Piezoelectricity, *Pyroelectricity, Heat transfer, Adiabatic conditions, Polyvinyl fluoride, Reprints, *Vinylidene fluoride polymers, Biomedicine.

Ferroelectric polymers such as polyvinylidene fluoride, polyvinyl fluoride, and several copolymers and blends when poled have pressure and temperature transduction properties which are related mainly to volume changes. Because of compressional heating effects, the pressure response includes both piezoelectric and pyroelectric terms, the latter representing nominally a -10 percent effect under adiabatic conditions. At low frequencies, where there is enough time in a cycle period for significant heat to be exchanged between the polymer and the surroundings becomes relevant as well as the compressional heating of the surroundings. For sensors in good thermal contact with thermally conducting surroundings, the time constant for internal thermal equilibration of the polymer becomes relevant also along with the polarization distribution function, unless the latter is uniform. The piezoelectric response of thin tubes, balloons and caps is discussed within the dipole density model for which the response is determined by thickness changes.

500,263
PB85-205300 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Molecular Spectroscopy Div.

Two-Photon Induced Fluorescence of the Tumor Localizing Photosensitizer Hematoporphyrin Derivative via 1064 NM Photons from a 20 NS Q-Switched Nd-YAG Laser.

Final rept.,
R. Bodaness, and D. King. 16 Jan 85, 6p
Pub. in Biochemical and Biophysical Research Communications 126, n1 p346-351, 16 Jan 85.

Keywords: *Fluorescence, *Hematology, *Porphyrins, *Photochemical reactions, *Chemotherapy, Biochemistry, Excitation, Photons, Reprints, *Cancer, Laser applications.

The authors demonstrate the direct 1064 micrometers two-photon excitation of hematoporphyrin derivative (HPD), a complex mixture of photosensitizing porphyrins which is selectively retained in tumor tissue and used in cancer photochemotherapy. Although 1064 micrometers is outside of the one-photon HPD absorption spectrum, two-photon induced fluorescence from HPD was observed following excitation by the 20 ns output of an amplified, Q-switched Nd-YAG laser at peak power levels of 0.1 to 3 GW/sq cm. Evidence for the successful two-photon excitation to vibrational levels of the S1 state consists of the observation of the known HPD fluorescence spectrum exhibiting peaks at approximately 615 and 675 micrometers, with the observed two-photon induced fluorescence intensity exhibiting a quadratic dependence on the excitation laser intensity as required for a direct two-

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Group 7D—Physical Chemistry

photon process. More generally, these results suggest the possibility for the achievement of photosensitized oxidations utilizing photons of lower energy than that required for single photon excitation, offering the potential for both greater selectivity and a reduction in competing photochemical processes.

500,264
PB85-205342 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.
SANS (Small-Angle Neutron Scattering) and SAXS (Small-Angle X-ray Scattering) Studies on Molecular Conformation of a Block Polymer in Microdomain Space.
Final rept.,
H. Hasegawa, T. Hashimoto, H. Kawai, T. P. Lodge, and E. J. Amis. 1985, 12p
Pub. in *Macromolecules* 18, n1 p67-78 1985.

Keywords: *Neutron scattering, *X ray analysis, *Polymers, Polystyrene, Polyisoprene, Reprints, *Molecular conformation, *Small angle scattering.

The molecular conformation of a block polymer chain in a microphase-separated domain space (a confined space) was studied by small-angle neutron scattering (SANS) with a deuterium labeling technique. The samples studied were polystyrene-polyisoprene diblock polymers, and they have a morphology of highly oriented alternating lamellar microdomains composed of polystyrene (PS) and polyisoprene (PI) in bulk when cast from dilute solutions in toluene. Conclusion (iii) does not mean at all that the chains in domain space are unperturbed but rather that they are strongly perturbed. The lateral contraction was proposed to be the consequence of the repulsive potential between the centers of block chains which are located in narrow interfacial regions (i.e., essentially in the two-dimensional space). A residual 'memory' of the repulsion in the bulk block polymer could be a consequence of the two-dimensionality of the space available to chemical junctions of the block polymers and/or an effect of repulsive potential (which existed in the polymer solution with a good solvent) being 'locked-in' at high polymer concentrations.

500,265
PB85-205631 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Ionization Energies and Entropies of Cycloalkanes: Kinetics of Free Energy Controlled Charge-Transfer Reactions.
Final rept.,
L. W. Sieck, and M. Mautner. 1982, 5p
Pub. in *Jnl. of Physical Chemistry* 86, n18 p3646-3650 1982.

Keywords: *Cyclohexanes, *Reaction kinetics, *Free energy, *Ionization, Chemical equilibrium, Mass spectroscopy, Enthalpy, Entropy, Thermodynamic properties, Reprints.

Enthalpies and entropies of ionization (ΔH ion and ΔS ion) of alkylcyclohexanes, as well as cycloheptane, cyclooctane, and trans-decalin, have been determined by charge transfer equilibrium measurements. A major effect of alkyl substitution is observed following substitution at a site alpha to a tertiary hydrogen atom (as from methyl-cyclohexane to 1,2-dimethylcyclohexane), or following replacement of a tertiary hydrogen atom (as from methylcyclohexane to 1,1-dimethylcyclohexane). The charge transfer reactions involving the cycloalkanes are shown to be fast processes; i.e., the sum of the reaction efficiencies ($r = k/k(\text{collision})$) of the forward and reverse processes is near unity. The efficiencies of these processes appear to be determined uniquely by the overall free energy change (or equilibrium constant K).

500,266
PB85-205656 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Catalysis by Carbides, Nitrides and Group VIII Intermetallic Compound.
Final rept.,
S. T. Oyama, and G. L. Haller. 1982, 33p
Pub. in *Catalysis* 5, p333-365 1982.

Keywords: *Catalysis, *Carbides, *Nitrides, *Group 8 compounds, *Intermetallics, Physical properties, Chemical properties, Decomposition, Reaction, Oxidation, Hydrogenation, Isomerization, Hydrolysis, Ammonia, Reprints, Fischer Tropsch synthesis.

A review is presented of catalysis by carbides, nitrides, and Group VIII intermetallic compounds. The catalytic

and other properties of transition-metal carbides and nitrides are discussed for oxidation, hydrogenation, dehydrogenation, isomerization, hydrolysis, Fischer-Tropsch synthesis, and ammonia synthesis. A similar discussion is presented for catalysis by binary compounds of Group VIII metals and lanthanides or actinides. It is not clear at this time whether the unique properties of the latter catalysts are due to the method of preparation (e.g., the extent of decomposition) or to a particular metal-oxide interaction.

500,267
PB85-205664 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Bond Homolysis in High Temperature Fluids.
Final rept.,
S. E. Stein, D. A. Robaugh, A. D. Alfieri, and R. E. Miller. 1982, 4p
Pub. in *Jnl. of the American Chemical Society* 104, n24 p6567-6570 1982.

Keywords: *Reaction kinetics, *High temperature tests, *Fluids, Vapor phases, Liquid phases, Solutions, Chemical bonds, Chemical reactions, Reprints, *Ethane/diphenyl, *Free radicals, *Homolysis, *Cage effect(Chemistry).

Rate constants for the homolysis of 1,2-diphenylethane have been determined in tetralin, in dodecahydrotriphenylene and in the gas phase at temperatures above 350°C. The Arrhenius expression for this reaction in the gas phase has been found consistent with available thermo-kinetic data. In liquid tetralin up to its critical temperature and in liquid dodecahydrotriphenylene Arrhenius parameters for this reaction were found to be distinctly higher than gas phase values and rate constants to be somewhat lower. Differences between gas and liquid phase kinetics are attributed to recombination of nascent free radicals in solution (the 'cage effect'), the probability of which decreases with decreasing viscosity.

500,268
PB85-205706 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Dielectric Saturation and Dielectric Friction in Electrolyte Solutions.
Final rept.,
P. J. Stiles, J. B. Hubbard, and R. F. Kayser. 1982, 8p
Pub. in *Jnl. of Chemical Physics* 77, n12 p6189-6196 1982.

Keywords: *Dielectric properties, *Ion currents, *Electrolytes, Solutions, Electrohydrodynamics, Comparison, Experimental design, Reprints, Numerical solution.

Electrohydrodynamic equations developed by Hubbard and Kayser to account for the combined effects of dielectric saturation and dielectric friction on ionic motion in polar solvents are solved numerically to yield ionic conductances. Dielectric saturation is incorporated into this continuum treatment through a phenomenological relationship between the electric permittivity and field strength. The results of the analysis are critically tested by comparison with experimental conductance data.

500,269
PB85-205722 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Laser Intensity Dependence of Multiphoton Excitation vs. Collisional Relaxation in Chlorodifluoromethane and Chlorotrifluoroethylene.
Final rept.,
J. C. Stephenson, J. A. Blazy, C. Li, and D. S. King. 1982, 6p
Pub. in *Jnl. of Chemical Physics* 76, n12 p5989-5994 1982.

Keywords: *Molecular relaxation, Excitation, Reprints, *Methane/chloro-difluoro, *Ethylene/chloro-trifluoro, *Laser induced fluorescence, *Multiphoton processes, *Molecular photon interactions.

CO₂ laser pulses for which the intensity vs. time profile is rectangular (10 or 50 ns duration) were used in the multiphoton excitation of CF₂HCl and CF₂CFCl dilute in high pressure (400 Torr) argon. Energy deposition was measured by optoacoustic detection, and CF₂ product yield by laser-excited fluorescence. Even at low yield (e.g. .001) more than 100 photons were absorbed per CF₂CFCl molecule, while for an identical yield, CF₂HCl absorbed 200 times less energy. For the same laser fluorescence, the higher intensity 10 micro-

seconds pulses gave more yield from CF₂CFCl (factors up to 500 were observed) than the less intense 50 microseconds pulses: for CF₂HCl the two intensities give the same yield. For both molecules, the two intensities gave the same optoacoustic signal for a given fluorescence. These results are related to the dependence on reactant energy of the competing ratio of collisional deactivation to laser excitation.

500,270
PB85-205730 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Photon Stimulated Desorption of Ions from Water and Methanol Adsorbed on a Titanium(0001) Surface.
Final rept.,
R. Stockbauer, D. M. Hanson, S. A. Flodstrom, E. Bertel, and T. E. Madey. 1983, 3p
Pub. in *Physica Scripta* 4, p126-128 1983.

Keywords: *Desorption, *Ions, Simulation, Water, Carbinols, Titanium, Surface chemistry, Reprints.

Synchrotron radiation has been used to study ion desorption from water and methanol adsorbed on a Ti(0001) surface, in an effort to understand ion desorption from covalently bonded systems. Both water and methanol dissociate upon adsorption on Ti at 300K. Using variable wavelength UPS, the species OH, O and H are observed for water and CH₃O, C, O and H for methanol. No molecular species adsorb at 300K. At 90K, dissociation occurs initially to yield the same products, while at higher exposures, condensed overlayers are formed. PSD of ions from the two adsorbates show very different behavior. In the water experiment ion desorption is dominated by the dissociated species at both 300 and 90K. H(+) emission from dissociated water is correlated with the presence of OH on the surface while ion desorption from the ice multilayer is almost an order of magnitude less. In contrast, ion emission from the dissociated methanol is immeasurably low in our instrument while a large H(+) signal is observed from the condensed layer.

500,271
PB85-205771 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Surface Raman Scattering from Effervescent Magnetic Peroxyborates.
Final rept.,
G. E. Walrafen, P. N. Krishnan, D. L. Griscom, R. G. Munro, and M. Hokmabadi. 1982, 7p
See also AD-A116899.
Pub. in *Jnl. of Chemical Physics* 77, n8 p3840-3846 1982.

Keywords: *Raman spectra, *Reaction kinetics, *Catalysis, *Oxygen, Surface chemistry, Concentration(Composition), Reprints, *Trapped particles, *Boric acid/peroxy-(sodium-salt).

Raman spectra were obtained from NaBO₃(4H₂O) and NaBO₃(H₂O), from electron bombarded peroxyborates from peroxyborated heated for various times and at temperatures from 110-180°C and from solid Na₂O₂ and BaO₂. The Raman spectra indicate that the breakdown of peroxy groups is accompanied by the formation of trapped molecular O₂. Quantitative Raman intensity data were also obtained as functions of heating time at 110°C for the 1556/cm lines whose intensities scale with the peroxy concentration. These intensity data were treated by logistics theory, and they were found to be consistent with a second-order autocatalyzed forward reaction dependent on the product of the peroxy and trapped O₂ concentrations, plus a first-order reverse reaction dependent upon the trapped O₂ concentration.

500,272
PB85-205789 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Interpretation of Quasi-Elastic Light Scattering Data for Flexible Chains: Model Dependence.
Final rept.,
P. H. Verdier, and D. E. Kranbuehl. 1983, 4p
Pub. in *Polymer* 24, n4 p383-386 1983.

Keywords: *Light scattering, *Mathematical models, *Elastic scattering, *Polymers, Dynamics, Molecular structure, Polarizability(Charge separation), Reprints, Polymer chains.

The autocorrelation functions and corresponding relaxation times obtained from the forward depolarized quasi-elastic light scattering experiment are exhibited

for two quite similar models of flexible polymer chains in solution. A very small change in the chain dynamics is found to be sufficient to change the relaxation time from a relatively short time independent of chain length, with an autocorrelation function suggestive of an unweighted sum of contributions from all the relaxation times in the spectrum of chain motion, to a long time with an autocorrelation function identical with those for the end-to-end vector, strongly dependent upon chain length and dominated by the longest relaxation time in the spectrum. These results raise the question whether widely-used models in which information about short-range chain structure and motion is deliberately omitted can be expected to be appropriate for the interpretation of depolarized scattering experiments.

500,273
PB85-205821 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.

Delta-Band Bonding Theory of the Relative Heats of Solution of Transition Metal Alloys and Its Relation to Solubility Limits.

Final rept.,
R. E. Watson, L. H. Bennett, and D. A. Goodman.
1983, 7p
Pub. in *Acta Metallurgica* 31, n8 p1285-1291 1983.

Keywords: *Transition metals, *Solubility, *Alloys, Heat of formation, Chemical bonds, Reprints.

The relative solubilities of one transition metal in another, and vice-versa, are derived within a Friedel d-band bonding model. The results are found to be in accord with experiment.

500,274
PB85-205839 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.

Regime III Crystallization in Melt-Crystallized Polymers: The Variable Cluster Model of Chain Folding.

Final rept.,
J. D. Hoffman. 1983, 24p
Pub. in *Polymer* 24, n1 p3-26 1983.

Keywords: *Crystal growth, *Nucleation, *Reaction kinetics, Crystallization, Polyethylene, Acetal resins, Reprints, *Polymer chains, *Variable cluster model, Poly(methylene/oxy), Polycrystalline compounds.

The kinetic nucleation theory of chain folding, including the effects of reptation, is extended to predict the increase in crystal growth rate G that is implied by measurements on PE and POM at moderately large undercoolings. Growth rate data on PE and POM crystallized from the melt suggest conformity with the theoretical predictions. The implications of Regime III crystallization to chain morphology are discussed.

500,275
PB85-205847 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.

Recent Developments in the Theory of Electron Scattering by Highly Polar Molecules.

Final rept.,
D. W. Norcross, and L. A. Collins. 1982, 57p
Pub. in *Advances in Atomic and Molecular Physics* 18, p341-397 1982.

Keywords: *Electron scattering, Polarity, Reprints, *Electron molecule interactions.

Theoretical and computational techniques for electron-collisions with polar molecules are reviewed. Particular problems addressed are the availability of simple perturbative approaches and the use of the fixed-nuclei approximation.

500,276
PB85-205870 Not available NTIS
National Bureau of Standards (NML), Boulder, CO.
Quantum Physics Div.

Ab Initio Calculation of Spectroscopic Properties of SiO and HOSi(+).

Final rept.,
P. Botschwin, and P. Rosmus. 1 Feb 85, 7p
Sponsored by Deutsche Forschungsgemeinschaft, Bonn-Bad Godesberg (Germany, F.R.).
Pub. in *Jnl. of Chemical Physics* 82, n3 p1420-1426 Feb 85.

Keywords: *Spectroscopic analysis, *Silicon monoxide, *Silicon oxides, Dipole moments, Vibrational spectra, Rotational spectra, Reprints, *Proton affinity.

Spectroscopic properties of SiO and HOSi(+1) have been calculated from highly correlated wave functions.

While the dipole moment of HOSi(+1) is very small (which will make detection of pure rotational transitions of this ion a difficult task), large intensities are predicted for stretching vibrational transitions both in absorption and emission. The proton affinity of silicon monoxide is calculated to be 8.44 eV.

500,277
PB85-205888 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.

Ab Initio Effective Spin-Orbit Operators for Use in Atomic and Molecular Structure Calculations. Results for Methylidyne, Hydroxyl Radicals, Silyldiyne, Carbon Monoxide(+1) Ion, Carbon Monoxide and Silicon Monoxide.

Final rept.,
W. J. Stevens, and M. Krauss. 1982, 3p
Pub. in *Jnl. of Chemical Physics* 76, n7 p3834-3836 1982.

Keywords: *Atomic structure, *Molecular structure, *Spin orbit interactions, Carbon monoxide, Ions, Comparison, Reprints, *Ab initio analysis, Silicon monoxide, Silyldiyne, Methylidyne, Hydroxyl radicals.

Ab initio effective spin-orbit operators, based on relativistic effective core potentials are used to determine the spin-orbit coupling constants for CH(X(sup 2) pi(sub r)), OH(X(sup 2) pi(sub i)), SiH(X(sup 2) pi(sub r)), CO(+1)6(A(sup 2) pi(sub i)), CO(A(sup 3) pi(sub r)), and SiO(A(sup 3) pi(sub r)). Comparison with experimental values and ab initio all electron values are very favorable.

500,278
PB85-205896 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.

Thermodynamic Properties of isobutane for Temperatures from 250 to 600 K and Pressures from 0.1 to 40 MPa.

Final rept.,
M. Waxman, and J. S. Gallagher. 1983, 18p
Pub. in *Jnl. of Chemical and Engineering Data* 28, n2 p224-241 1983.

Keywords: *Thermodynamic properties, Tables(Data), Pressure, Density(Mass/volume), Surfaces, Temperature, Reprints, *Virial coefficients, *Propane/methyl.

Tables of isobutane thermodynamic properties are presented for temperatures from 245 to 600 K and pressures from 0.1 to 40 MPa. The tables include saturation and isobaric properties; namely, pressure, specific volume, temperature, internal energy, enthalpy and entropy. The properties are defined by a specific thermodynamic surface, which is expressed analytically in the form of the Helmholtz energy as a function of temperature and density. The surface is developed from only pressure-density-temperature data. The appendix to the paper includes a summary of the correlation development and of new isobutane measurements, saturated vapor pressures and isothermal pressure-density-temperature data for temperatures of 377.59, 394.26, 423.15 and 448.15 K. The isothermal data are reported in the form of a virial series representation of the compressibility factor for pressures up to about 3.5 MPa and as correlated Burnett points for the higher pressures at 423.15 K. The data were used to assess the reliability of literature sources used in the correlation. Surface derived properties are compared with experimental data.

500,279
PB85-205938 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.

Laser Spectroscopy and Chemiluminescence from the Monomethoxides of Calcium, Strontium, and Barium.

Final rept.,
R. F. Wormsbecher, and R. D. Suenram. 1982, 14p
Pub. in *Jnl. of Molecular Spectroscopy* 95, n2 p391-404 1982.

Keywords: *Chemiluminescence, *Vibrational spectra, Chemical bonds, Molecular structure, Reprints, *Laser spectroscopy, *Calcium methoxides, *Strontium methoxides, *Barium methoxides.

Production of the monomethoxides of Ca, Sr, and Ba (MOCH₃) is described. The production scheme uses a metal vapor flow reactor in which the appropriate metal vapor is mixed with methyl nitrite (CH₃ONO) to produce the metal methoxides. Chemiluminescence spectra from these reactions is recorded, and features due the metal oxides, and mono-methoxide are observed. Dynamical aspects of these reactions are dis-

cussed. Laser excitation spectra are obtained for CaOCH₃, CaOCD₃, SrOCH₃, SrOCD₃, using a pulsed dye laser. Vibrational features are observed and assigned for all of the molecules. A summary of frequencies is given. The nature of the bonding and structural considerations of the monomethoxides are described in terms of a localized ionic bonding model which was used previously on the isoelectronic monohydroxides and monohalides of the alkaline-earth.

500,280
PB85-205953 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.

Identification of Lead Sources in California Children Using the Stable Isotope Ratio Technique.

Final rept.,
Y. Yaffe, C. P. Flessel, J. J. Wesolowski, A. del Rosario, and G. N. Guirguis. 1983, 9p
Pub. in *Archives of Environmental Health* 38, n4 p237-245 1983.

Keywords: *Lead(Metal), *Isotopic labeling, *Public health, *Children, *Blood analysis, Paints, Soil analysis, Sources, Mass spectroscopy, Concentration(Composition), California, Chemical analysis, Reprints, *Environmental health, Oakland(California), Case studies.

Two case studies applying the lead isotope ratio method to the identification of lead sources in twelve Oakland, CA children are presented. One study examined lead sources in ten children, ages 3 to 15 years, living together as an extended family in dilapidated housing close to a busy freeway. A second case study examined two-year old male twins, both with elevated blood lead and erythrocyte protoporphyrin levels, living in a modest but well maintained inner city duplex-apartment. Paint and surface soil samples collected in and around both households had high lead concentrations. The isotopic ratios of lead in the bloods of these children were close to the average lead ratios of paints from exterior walls and to the lead ratios of surface soils in adjacent areas where the children played. In both case studies, the data suggest that the lead in the soil was derived mainly from weathering of lead-based exterior paints and that the lead-contaminated soil was a proximate source of lead in the blood of the children.

500,281
PB85-205979 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Center for Materials Science.

JCPDS (Joint Committee on Powder Diffraction Standards) Data Base--Present and Future.

Final rept.,
W. Wong-ng, M. Holomany, W. F. McClune, and C. R. Hubbard. 1982, 2p
Sponsored by Denver Research Inst., CO.
Pub. in *Advances in X-Ray Analysis* 26, p87-88 1982.

Keywords: *X ray diffraction, *Powders, Reprints, Data bases, X ray powder diffraction, NBS-AIDS80 computer program.

The Powder Diffraction File is a large numerical data base consisting of nearly 40,000 x-ray powder diffraction patterns. This data base is being converted from the storage on Gothic cards to a magnetic form in order to simplify operations and to enhance product generation. The computer program NBS-AIDS80, which is being used to prepare the data base, also provides extensive, systematic methods of evaluating powder patterns.

500,282
PB85-205995 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.

SANS (Small Angle Neutron Scattering) Investigation into the Role of Melting and Recrystallization during Solid State Deformation of Polyethylene.

Final rept.,
G. D. Wignall, and W. Wu. 1983, 6p
Pub. in *Polym. Communic.* 24, n12 p354-359 1983.

Keywords: *Polyethylene, *Plastic deformation, *Neutron scattering, *Melting, *Crystallization, Molecular weights, Blends, Deuterium compounds, Reprints, *Small angle scattering, *Molecular conformation, *Solid state chemistry.

Small angle neutron scattering (SANS) has been used to investigate the role of melting and recrystallization in the solid state deformation of polyethylene. Blends containing 4.3 vol % deuteropolyethylene (PED) in normal polyethylene (PEH) have been prepared with

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non-random distribution of PED molecules in PEH. These blends show anomalously high apparent SANS molecular weights ($M(\text{sub } w)$) and radii of gyration, resulting from the correlations in the centers of gravity (clusters) of the PED molecules. A dramatic reduction in the SANS ($M(\text{sub } w)$) was observed in the specimens subject to plastic deformation in a temperature range (50-119°C) where annealing alone is known not to affect ($M(\text{sub } w)$). A similar reduction in the apparent SANS- $M(\text{sub } w)$ may be achieved by melting and rapidly quenching the blend. This implies that large scale reorganization takes place at the molecular level during deformation, with a consequent relative motion and randomization of the centers of gravity of the PED molecules. The implications of these findings are discussed in terms of the mechanisms involved in the plastic deformation process.

500,283

PB85-206001 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Model for the Saturated Water Bilayer on Ru(001) Based on a Comparison of Experimental and Calculated LEED Patterns.
Final rept.,
E. D. Williams, and D. L. Doering. 1983, 5p
Pub. in Jnl. of Vacuum Science and Technology A 2, n2 p1188-1192 1983.

Keywords: *Mathematical models, *Water, *Adsorption, *Surface chemistry, *Molecular structure, Electrolytes, Electrochemistry, Comparison, Experimental design, Ruthenium, Electron diffraction analysis, Chemical bonds, Reprints, *LEED (Low energy electron diffraction), Electron stimulated desorption ion angular distributions, Numerical solution, Thermal desorption.

A complex coverage- and temperature-dependent LEED pattern was observed for water adsorbed on clean Ru(001). This pattern has been modeled in terms of an antiphase structure of two-dimensional, hydrogen-bonded, bilayer domains. A computer simulation of the LEED patterns arising from this model structure gives good agreement with the experimental results. Other considerations in the model determination were based on simple water bilayer island models which were developed to explain experimental thermal desorption and electron stimulated desorption ion angular distribution data. This new insight into the molecular structure of adsorbed water on Ru may lead to a better understanding of the metal-electrolyte interface in electrochemistry.

500,284

PB85-206068 PC A06/MF A01
National Bureau of Standards, Gaithersburg, MD.
NBSGSC - A FORTRAN Program for Quantitative X-ray Fluorescence Analysis.
Technical note (Final),
G. Y. Tao, P. A. Pella, and R. M. Rousseau. Apr 85, 124p NBS/TN-1213
Also available from Supt. of Docs as SN003-003-02653-1. Prepared in cooperation with Geological Survey of Canada, Ottawa (Ontario).

Keywords: *X ray analysis, *Spectral energy distribution, *X ray fluorescence, Spectrometers, Chemical analysis, Oxides, Alloys, Minerals, Computation, Quantitative analysis, Fortran, Computer programs, Concentration (Composition), Standards, X ray tubes, Gamma radiation, *Alpha coefficients.

A FORTRAN program (NBSGSC) was developed for performing quantitative analysis of bulk specimens by x-ray fluorescence spectrometry. This program corrects for x-ray absorption/enhancement phenomena using the comprehensive alpha coefficient algorithm proposed by Lachance (COLA). NBSGSC is a revision of the program ALPHA and CARECAL originally developed by R.M. Rousseau of the Geological Survey of Canada. Part one of the program (CALCO) performs the calculation of theoretical alpha coefficients, and part two (CALCOMP) computes the composition of the analyte specimens. The analysis of alloys, pressed minerals, and fused specimens can currently be treated by the program. In addition to using measured x-ray tube spectral distributions, spectra from seven commonly used x-ray tube targets could also be calculated with an NBS algorithm included in the program. NBSGSC is written in FORTRAN IV for a Digital Equipment Corporation (DEC PDP-11/23) minicomputer using RLO2 firm disks and an RSX 11M operating system.

500,285

PB85-206456
(Order as PB85-206324, PC A13/MF A01)
Northwestern Univ., Evanston, IL.
Review of the Optical Data Analysis for Phthalocyanine Conducting Polymer and Molecular-Metal Systems.
W. J. McCarthy, C. R. Kannewurf, T. Inabe, T. J. Marks, and R. L. Burton. Apr 85, 4p
Prepared in cooperation with IIT Research Inst., Chicago, IL.
Included in OM85: Basic Properties of Optical Materials. Summaries of Papers, p54-57 Apr 85.

Keywords: *Phthalocyanines, *Metal containing organic compounds, *Optical tests, Reviews, Additives, Optical properties, Polycrystals, Dielectric properties, *Polyphthalocyanines, Doped materials.

During the past decade a number of interesting low-dimensional materials have been prepared which have been found to exhibit a combination of unusual properties that are not generally observed in the conventional inorganic semiconductor and metallic systems. Optical diagnostics have provided a key method for obtaining important information about both molecular-metal and conducting polymer systems. For many of these systems the optical measurements and the methods of analysis have been carried out by D.B. Tanner, C.S. Jacobsen and their respective co-workers. At this laboratory the principal effort in this area has been devoted to the development of phthalocyanine based systems with various doping agents. It has been found that the phthalocyanine polymers possess a rather unique blend of properties that show considerable promise for applications. Optical reflectance studies have also provided valuable information about the phthalocyanine systems, but for many compounds single crystal samples have not been successfully prepared as yet. Thus the majority of the optical measurements have been performed on polycrystalline pressed powder compactions. Such specimens also have been used to provide information in other systems that could not be obtained from single crystal data alone.

500,286

PB85-206464
(Order as PB85-206324, PC A13/MF A01)
Oak Ridge National Lab., TN.
Optical Properties of PBS (Poly(butene-1-sulfone)).
M. W. Williams, D. W. Young, J. C. Ashley, and E. T. Arakawa. Apr 85, 2p
Contract DE-AC05-84OR21400
Sponsored by Rome Air Development Center, Griffiss AFB, NY.
Included in OM85: Basic Properties of Optical Materials. Summaries of Papers, p58-59 Apr 85.

Keywords: *Optical properties, Photons, Electron energy, Lithography, Microstructure, *Polybutene sulfone.

PBS, or poly(butene-1-sulfone) with a formula of $(C_4H_8SO_2)_n$, is a fast electron-resist used in microlithography. To understand, and to be able to predict, the resolution attainable with this system, it is necessary to know the optical properties of the resist material over the range of photon energies associated with the oscillator strength of the valence electrons. Electron mean free paths in the material can be calculated from these data as a function of incident electron energy. Energy deposition and details of track structure can then be calculated for incident electron beams. Predictions of the sharpness and resolution in the resulting microstructures can be compared with those obtained experimentally.

500,287

PB85-206498
(Order as PB85-206324, PC A13/MF A01)
Illinois Univ. at Urbana-Champaign.
Quantitative Sampling in Planar Waveguides.
P. W. Bohn. Apr 85, 3p
Included in OM85: Basic Properties of Optical Materials. Summaries of Papers, p71-73 Apr 85.

Keywords: *Spectroscopic analysis, *Thin films, *Mathematical models, *Polymeric films, Raman spectra, Elastic scattering.

A simple model for quantitative spectroscopic sampling in thin films has been advanced and compared with experiment for the simple case of spatially homo-

geneous scatterers. Agreement with theoretical scattering intensities demands a treatment which takes into account both surface and volume elastic scattering and mode dependent coupling efficiency effects.

500,288

PB85-206696
(Order as PB85-206324, PC A13/MF A01)
Hughes Aircraft Co., Long Beach, CA.
Importance of Electron-Electron Correlation in the Calculation of Second-Order Nonlinear Optical Properties of Organic Molecules. The Case of Urea.
B. M. Pierce. Apr 85, 4p
Included in OM85: Basic Properties of Optical Materials. Summaries of Papers, p150-153 Apr 85.

Keywords: *Molecular structure, *Optical properties, *Organic compounds, Excitation, Molecular energy levels, *Electron electron interactions, *Nonlinear optics, *Self constant field molecular orbitals, *SCF MO methods, *Single excitation configuration interactions.

In studies of nonlinear optical organic molecules, the theoretical understanding of the relation between the electronic structure of the molecule and the molecular electronic component of the second-order nonlinear optical susceptibility (the hyperpolarizability tensor, β_{ijk}) has been an important objective (1). The theoretical description of molecular electronic structure improves with the theoretical treatment of electron-electron correlation (EEC) in the molecule. Three general quantum mechanical molecular orbital (MO) formalisms (2) used to study molecular electronic structure, and ordered according to an improving treatment of EEC, are (1) the self-consistent-field (SCF)-MO method, (2) the SCF-MO method with single excitation configuration interaction (SCF-MO-SCI), and (3) the SCF-MO method with single and double excitation configuration interaction (SCF-MO-SDCI). The organic molecule selected for the authors initial theoretical study was urea, $(NH_2)_2CO$, because its nonlinear optical response has been the subject of extensive theoretical and experimental investigations.

500,289

PB85-207124 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Precision X-ray Wavelength Measurements in Helium-Like Argon Recoil Ions.
Final rept.,
R. D. Deslattes, H. F. Beyer, and F. Folkmann. 1984, 6p
Pub. in Jnl. of Physics B: Atomic and Molecular Physics 17, pL689-L694 1984.

Keywords: *X ray analysis, *Ions, *Radioactive decay, Argon, Calibrating, Performance evaluation, Quantum electrodynamics, Wavelengths, Reprints, *Argon ions, *Ion ion collision.

The authors report precise wavelength measurements of the 1 double s $S(\text{sub } 0)-1s2p(\text{sup } 3)P(\text{sub } 12)$, transitions in $Ar(+16)$ produced by collisions of 5.9 MeV/amu $U(+66)$ ions with an argon gas target. By use of this 'recoil source', the precision is not limited by Doppler shifts while the influence of spectator electrons is minimized by observation of their relative importance as a function of gas pressure. The accuracy obtained is at the 12 ppm level dominated by the x-ray calibration standard. The measurement is thus sensitive to quantum-electro-dynamic (QED) and electron correlation effects.

500,290

PB85-207199 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Fluorescence Quenching of Liquid Alkylbenzenes Excited By Nonionizing and Ionizing Ultraviolet Radiation and By Beta-Radiation.
Final rept.,
F. P. Schwarz, and M. Mautner. 1983, 8p
Pub. in Jnl. of Physical Chemistry 87, n25 p5206-5213 1983.

Keywords: *Benzenes, *Ultraviolet radiation, *Beta particles, *Photoionization, Fluorescence, Excitation, Xylenes, Molecular energy levels, Cations, Reprints, *Fluorescent quench principle, Benzene, Benzene/propyl, Mesitylene, Indan, Decylbenzene, Ion electron collisions, Ion ion collisions.

At wavelengths above the photoionization wavelength, the CCl_3H quenching of the benzene, toluene, o-

xylylene, p-xylylene, mesitylene, propylbenzene, isopropylbenzene, indane, and decylbenzene fluorescences results from quenching of the S1 state with quenching constants ranging from 0.6 plus or minus 0.1 M(-1) for benzene to 19 plus or minus 1 M(-1) for p-xylylene. At wavelengths below the photoionization wavelength, the S1 fluorescence is generated from recombination of the aromatic cation-electron ion-pairs and the fluorescence yield increases to an average of 0.8 plus or minus 0.1 near 1450 Å for the alkylbenzene derivatives. The CCl₃H quenching of the recombination fluorescence results from quenching of the ion-pairs and the quenching constants increase from 0 near the estimated photoionization wavelength to a near constant value ranging from 3.0 plus or minus 0.2/M (mesitylene) to 1.7 plus or minus 0.2/M (indane) below 1450 Å.

500,291
PB85-207207 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Dioxin Formation in Incinerators.

Final rept.,
W. M. Shaub, and W. Tsang. 1983, 10p
Pub. in Environmental Science and Technology 17,
n12 p721-730 1983.

Keywords: *Mathematical models, *Air pollution, *Incinerators, Combustion products, Forecasting, Sources, Reprints, *Dioxin(Herbicides), *Polychlorinated dibenzodioxins, *Chemical reaction mechanisms, Numerical solution, Polychlorinated biphenyls, Homogeneous reactions.

Processes which may contribute to the formation of polychlorinated dibenzo-p-dioxins (PCDDs) are examined. A model mechanism has been constructed to investigate the possibility for homogeneous gas phase formation of PCDDs from polychlorinated phenols in an incinerator environment. Numerical calculations have been performed. The results lead to the conclusion that the probability for gas phase formation of PCDDs is likely to be very low at high temperatures if mixing between fuel and air is efficient. Effects of use of auxiliary hydrocarbon fuel and excess air are examined. Probable sources of non-idealities are examined. The potential role of non-gas phase effects is considered. Conclusions are drawn regarding some future research needs.

500,292
PB85-207272 Not available NTIS
National Bureau of Standards (NML), Boulder, CO.
Quantum Physics Div.

Measurement of Relative Extreme-Wing Absorption Coefficients By Excited-State Degenerate Four-Wave Mixing.
Final rept.,
P. Ewart, and S. V. O'Leary. Nov 84, 8p
Pub. in Jnl. of Physics B: Atomic and Molecular Physics 17, n22 p4609-4616 1984.

Keywords: Helium, Neon, Argon, Excitation, Reprints, *Absorption coefficients, *Sodium atoms, *Degenerate four wave mixing.

The population of the 3P state in atomic sodium produced by absorption in the extreme blue wing of the D lines is measured by excited state degenerate four-wave mixing (ESDFWM). The strength of the ESDFWM signal is shown to give a measure of the pressure-broadened extreme-wing absorption coefficient $\alpha(\omega)$. Relative values of $\alpha(\omega)$ for the rare gases He, Ne and Ar are measured and compared with values calculated from theoretical interatomic potentials and from extreme-wing emission data. Very good agreement is found demonstrating the ability of the nonlinear technique to make accurate measurements of small excited-state densities with excellent spatial and temporal resolution. Advantages of the method for other applications are briefly discussed.

500,293
PB85-207280 Not available NTIS
National Bureau of Standards (NML), Boulder, CO.
Quantum Physics Div.

Absorption and Saturation Effects on Degenerate Four-Wave Mixing in Excited States Formed during Collisions.
Final rept.,
P. Ewart, and S. V. O'Leary. Nov 84, 14p
Pub. in Jnl. of Physics B: Atomic and Molecular Physics 17, n22 p4595-4608 1984.

Keywords: Helium, Neon, Argon, Excitation, Reprints, *Degenerate four wave mixing, Sodium atoms, Laser radiation.

Degenerate four-wave mixing (DFWM) in excited atoms is investigated as a probe of the excited state density produced by collision assisted transitions. Sodium atoms are excited to the 3P state by absorption of light in the extreme blue wing of the D lines in the presence of He, Ne and Ar perturbers. The rare gas-pressure dependence of the DFWM signals, resonantly enhanced by the 3P-4D transition, is studied to determine the regime where the signals give an unambiguous measure of the excited state (3P) density. The observed behavior is compared with a simple model of DFWM in absorbing media. Good qualitative agreement is obtained and the results illustrate the role of absorption, saturation and finite laser bandwidth. The technique allows small excited state densities (about 10 to the 9th power/cc) to be detected with good temporal and spatial resolution.

500,294
PB85-207298 Not available NTIS
National Bureau of Standards (NML), Boulder, CO.
Quantum Physics Div.

Electron-ion ionization.
Final rept.,
G. H. Dunn. 1985, 43p
Pub. in Electron Impact Ionization, Chapter 8, p277-319 1985.

Keywords: *Ionization, *Reaction kinetics, *Cross sections, Ions, Reviews, Excitation, Experimental design, Reprints, *Chemical reaction mechanisms, *Electron-ion collisions, *Electron impact spectra, Autoionization.

Methods are presented for measurement of rates and cross sections for electron-impact ionization of ions. Status of the data is reviewed. Specific data are discussed and compared with various theoretical estimates. The ionization mechanisms of direct ionization, excitation-autoionization, and resonant excitation-double autoionization are demonstrated with specific examples from the measured data.

500,295
PB85-207322 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.

Study of Polycation-Anionic-Surfactant Systems.
Final rept.,
P. S. Leung, and E. D. Goddard. 1985, 16p
Pub. in Colloids and Surfaces 13, p47-62 1985.

Keywords: *Polyelectrolytes, *Cations, *Anions, *Surfactants, *Neutron scattering, Copolymers, Molecular structure, Viscosity, Vinyl copolymers, Stability, Reprints, *Sulfuric acid/dodecyl-(sodium-salt), *Small angle scattering, *Molecule molecule interactions, *Ion molecule interactions, Polymer chains, Cellulose ether.

An investigation of the interaction of sodium dodecyl sulfate (SDS) with two cationic polyelectrolytes, Polymer JR, a cationic cellulose ether, and Reten, a synthetic vinyl copolymer, is reported. The study emphasizes small angle neutron scattering but also includes viscosity and dye-solubilization measurements. The results indicate that small additions of SDS to Polymer JR of 1% concentration lead to intermolecular interactions between the polymer chains via the bound surfactant, whereas in the more flexible and globular vinyl polyelectrolyte, intramolecular interaction is favored. Just into the resolubilization zone, where excess anionic surfactant is present (approximately 1.5% SDS), Polymer JR favors a polymer micellar association, whereas the more flexible Reten polymer seems to stabilize a structure involving association of surfactant into smaller units, perhaps surfactant pairs. In both cases the characteristic interaction peak of SDS micelles is absent in the SANS profile. When the surfactant is in large excess (5%) this peak returns, i.e., micellar structures predominate in both systems, probably with the macromolecule woven into the micellar domains, resembling an entangled string of beads.

500,296
PB85-207397 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Gas and Particulate Science Div.

Gravimetric Technique for the Preparation of Accurate Trace Organic Gas Standards.
Final rept.,
G. C. Rhoderick, W. F. Cuthrell, and W. L. Zielinski. 1985, 8p
Sponsored by Air Pollution Control Association, Pittsburgh, PA. and American Society for Quality Control, Inc., Milwaukee, WI.

Pub. in Proceedings of APCA/ASQC (Air Pollution Control Association/American Society for Quality Control) Speciality Conf. on Quality Assurance in Air Pollution Measurements, Boulder, Co., October 14-18, 1984, p239-246 1985.

Keywords: *Trace elements, *Gravimetric analysis, *Standards, *Hazardous materials, *Organic compounds, Chemical analysis, Concentration(Composition), *Air pollution detection.

An accurate procedure based on micro-gravimetry has been used for the preparation of volatile, hazardous organic chemicals in a nitrogen matrix in pressurized gas cylinders at analyte concentrations ranging from 10 ppb to 10 ppm, by mole. In this technique, the organics of interest are individually weighed into separate glass capillary tubes using a micro-analytical balance. A number of these gravimetric primary mixtures have been prepared and analytically intercompared using gas chromatography (GC) with flame-ionization detection (FID). The paper will focus on a description of the micro-gravimetric technique and the analytical system, and will discuss the estimation of specific uncertainties associated with the preparation of these mixtures and how these uncertainties are used to assign a net uncertainty to the final analyte concentration. Particular attention will be given to mixtures at the 10 to 150 ppb level. A brief description of how the overall network of gravimetric primary standards is used to provide data quality consistency for trace organic gas mixtures over the long-term is included.

500,297
PB85-207439 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Inorganic Analytical Research Div.

Systematics of Multielement Determination with Resonance Ionization Mass Spectrometry and Thermal Atomization.

Final rept.,
L. J. Moore, J. D. Fassett, and J. C. Travis. Dec 84, 6p
Pub. in Analytical Chemistry 56, n14 p2770-2775 Dec 84.

Keywords: *Chemical analysis, Mass spectroscopy, Metastable state, Excitation, Atomizing, Photoionization, Atomic energy levels, Reprints, *Laser spectroscopy, *Thermal atomization, *Resonance ionization spectroscopy.

The systematics for multielement determination using resonance ionization mass spectrometry and thermal atomization is developed. The aspects of atomization, ionization, and detection are discussed and resonance ionization is demonstrated for 19 elements. The selective, sequential ionization of seven elements from a single sample is also demonstrated. A one-wavelength, two-photon ionization scheme generally is used in which the first photon excites a bound transition in the near-ultraviolet region and second photon promotes the electron into the ionization continuum. The wavelength-dependent ion formation from the thermally produced atom reservoirs is demonstrated for these elements by scanning a Nd: YAG-pumped dye laser across its tunable wavelength range. The observed wavelengths where ionization occurs have been correlated where possible with allowed transitions between known electronic energy levels. The elements accessible by using four common dyes are tabulated. More than 20 elements are accessible within the wavelength of each dye.

500,298
PB85-208056 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymer Science and Standards Div.

Viscoelastic Relaxation of Cross-Linked Polymer Networks.

Final rept.,
R. J. Gaylord, and E. A. DiMarzio. 1984, 4p
Pub. in Polymer Bulletin 12, p29-32 1984.

Keywords: *Elastomers, *Crosslinking, *Viscoelasticity, *Molecular relaxation, Entropy, Stress relaxation tests, Reprints, *Polymer chains.

Theoretical interpretations of the viscoelastic relaxation behavior of cross-linked elastomers are discussed. The dangling chain retracing mechanisms of de Gennes and Pearson-Helfand, which assume that the stress contribution of a dangling chain decreases as it assumes successively lower entropy configurations, are replaced by an alternative relaxation mechanism.

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nism, based on the hopping model of hindered diffusion.

500,299

PB85-208072

Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymer Science and Standards Div.

Monte Carlo Studies of Two Measures of Polymer Chain Size as a Function of Temperature.

Final rept.,

C. M. Guttman. Sep 84, 17p

Pub. in Jnl. of Statistical Physics 36, n5/6 p717-733 Sep 84.

Keywords: *Monte Carlo method, *Temperature, Radius of gyration, Reprints, *Polymer chains.

Monte Carlo simulations of single polymer chains with both excluded volume and nearest-neighbor interaction energies are discussed. Two measures of chain size are obtained in the simulation, the radius of gyration of the polymer chain and the inverse radius of the polymer chain. Both of these are reported as a function of temperature, or interaction energy, and chain length, N . The possibility of estimating the fractal dimensions of these measures from the Monte Carlo data is discussed in the context of two different interpolation functions for the temperature dependence of the fractal dimensions. The approach to the fractal dimension as a function of chain length, N , is studied. It is suggested that the approach to fractal dimension of the measures of chain size of polymers is slow, perhaps a fractional power itself.

500,300

PB85-219830

Not available NTIS
American Chemical Society, Washington, DC.

Journal of Physical and Chemical Reference Data, Volume 13, Number 4, 1984.

Quarterly rept.

c1984, 460p

See also PB85-219848 through PB85-219913 and PB85-137842. Sponsored by National Bureau of Standards, Washington, DC. Prepared in cooperation with American Inst. of Physics, New York.

Available from American Chemical Society, 1155 Sixteenth St., N.W., Washington, DC 20036.

Keywords: *Research projects, Assessments, Alkanes, Thermodynamic properties, Physical properties, Chemical properties, Molecular energy levels, Molecular vibration, Polymers, Electrical resistivity, Hafnium, Molybdenum, Tantalum, Tungsten, Elements, Reviews, Vanadium, Zirconium, Aluminum, Manganese, Zinc, Standards, Reaction kinetics, Copper, Specific heat, Photochemical reactions, *Reference materials, Matrix isolation technique, Atmospheric chemistry, Electron ion interactions.

Contents:

- Ground-state vibrational energy levels of polyatomic transient molecules;
- Electrical resistivity of selected elements;
- Electrical resistivity of vanadium and zirconium;
- Electrical resistivity of aluminum and manganese;
- Standard chemical thermodynamic properties of alkane isomer groups;
- Evaluated theoretical cross-section data for charge exchange of multiply charged ions with atoms. III. Nonhydrogenic target atoms;
- Heat capacity of reference materials: Cu and W;
- Evaluated kinetic and photochemical data for atmospheric chemistry;
- Supplement II. CODATA task group on gas phase chemical kinetics.

500,301

PB85-219848

Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Molecular Spectroscopy Div.

Ground-State Vibrational Energy Levels of Polyatomic Transient Molecules,

M. E. Jacox. c1984, 125p

Included in Jnl. of Physical and Chemical Reference Data, v13 n4 p945-1068 1984. Available from American Chemical Society, 1155 Sixteenth St., N.W., Washington, DC 20036.

Keywords: *Molecular energy levels, *Molecular vibration, *Polyatomic molecules, *Spectroscopic analysis, Tables(Data), Thermodynamic properties, Hydrides, Experimental design, Reaction kinetics, Van der Waals equations, Nitrogen, Argon, Neon, Chemical bonds, Photochemistry, Hydrocarbons, Temperature, Ultra-

violet spectroscopy, Infrared spectroscopy, *Laser spectroscopy, Matrix isolation techniques.

The experimentally determined ground-state vibrational energy levels of approximately 480 covalently bonded transient molecules possessing from 3 to 16 atoms are tabulated, together with references to the pertinent literature. The types of measurement surveyed include laser-based high resolution gas phase infrared absorption and visible-ultraviolet emission techniques, ultraviolet photoelectron spectroscopy, and matrix isolation spectroscopy. An assessment of the magnitude of the uncertainty of observations in neon, argon, and nitrogen matrices is given.

500,302

PB85-219889

Not available NTIS
Massachusetts Inst. of Tech., Cambridge. Dept. of Chemistry.

Standard Chemical Thermodynamic Properties of Alkane Isomer Groups,

R. A. Alberty, and C. A. Gehrig. c1984, 25p

Sponsored by National Bureau of Standards, Gaithersburg, MD.

Included in Jnl. of Physical and Chemical Reference Data, v13 n4 p1173-1197 1984. Available from American Chemical Society, 1155 Sixteenth St., N.W., Washington, DC 20036.

Keywords: *Alkanes, *Thermodynamic properties, *Standards, *Molecular isomerism, *Hydrocarbons, Stereochemistry, Chemical equilibrium, Fuels, Tables(Data), Temperature, Enthalpy, Entropy, Specific heat, Gibbs free energy, *Stereoisomers, *Benson method, Numerical solution.

The chemical thermodynamic properties of alkane isomer groups from C₄H₁₀ to C₁₀H₂₂ have been calculated from 200 to 1500 K from Scott's tables of 1974. The numbers of stereoisomers in each isomer group have been checked and all of them have been included in the calculations. The following properties for alkane isomer groups have been calculated with energy in joules for a standard state pressure of 1 bar; standard heat capacity at constant pressure, standard entropy, standard enthalpy of formation, standard Gibbs energy of formation, standard enthalpy relative to isomer group at 298.15 K, and standard enthalpy relative to the elements at 298.15 K. Equilibrium mole fractions within isomer groups have been calculated for the ideal gas state from 200 to 1500 K. The four basic properties are given for all the individual isomers in joules for a standard state pressure of 1 bar. The properties of individual alkanes from C₄H₁₀ to C₁₀H₂₂ have also been calculated using the Benson group method and the resulting isomer group properties and equilibrium mole fractions have been calculated.

500,303

PB85-219897

Not available NTIS
Joint Inst. for Lab. Astrophysics, Boulder, CO.

Evaluated Theoretical Cross-Section Data for Charge Exchange of Multiply Charged Ions with Atoms. 3. Nonhydrogenic Target Atoms,

R. K. Janev, and J. W. Gallagher. c1984, 49p

Sponsored by National Bureau of Standards, Gaithersburg, MD.

Included in Jnl. of Physical and Chemical Reference Data, v13 n4 p1199-1249 1984. Available from American Chemical Society, 1155 Sixteenth St., N.W., Washington, DC 20036.

Keywords: *Electron capture, *Electron transfer, Ion exchanging, Atomic energy levels, Assessments, Mathematical models, Collisional energy transfer, Experimental design, Graphs(Charts), Atoms, Ions, Tables(Data), *Atom ion interactions, *Ion ion interactions, *Charge exchange reactions, *Charge transfer cross sections, Numerical solution, Ion-atom collisions.

The theoretical cross-section data for single-electron capture in collisions of multiply charged ions with nonhydrogenic atoms are compiled and their accuracy is assessed. The energy per unit mass range considered is from about 1 eV/u to several MeV/u, u being the unified atomic mass unit. Accuracy is assessed using both pure theoretical arguments and comparison with experimental data, where available. A similar assessment is performed for the two-electron capture cross-section data in ion-atom collisions, as well as for single- and double-charge exchange in ion-ion collisions.

500,304

PB85-219905

Not available NTIS

Commonwealth Scientific and Industrial Research Organization, Lindfield (Australia). Div. of Applied Physics.

Heat Capacity of Reference Materials: Cu and W,

G. K. White, and S. J. Collocott. c1984, 5p

Sponsored by National Bureau of Standards, Gaithersburg, MD.

Included in Jnl. of Physical and Chemical Reference Data, v13 n4 p1251-1257 1984. Available from American Chemical Society, 1155 Sixteenth St., N.W., Washington, DC 20036.

Keywords: *Copper, *Specific heat, *Tungsten, Tables(Data), Purity, Pressure, Temperature, Thermodynamic properties, Measuring instruments, Metals, Interpolation, *Reference materials.

The CODATA Task Group on Thermophysical Properties is preparing a set of recommended values for the heat capacity, thermal expansion, and transport properties of key solids which are used in calibrating or checking measuring equipment. The present paper surveys selected data on heat capacity at constant pressure C_p of copper from 1 to 1300 K and tungsten from 1 to 3400 K. Selected values are tabulated for C_p and also for heat capacity at constant volume C_v . Interpolating functions are given for C_p .

500,305

PB85-221851

Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.

Photoionization of the H Atom in Strong Electric Fields by Resonant Two-Photon Excitation.

Final rept.,

K. H. Welge, and H. Rottke. 1984, 7p

Sponsored by Optical Society of America, Washington, DC.

Pub. in Proceedings of Topical Meeting on Laser Techniques Extreme Ultraviolet (2nd), Boulder, CO., March 5-7, 1984, American Institute of Physics Conference Proceedings 119, p213-219 1984.

Keywords: Ultraviolet lasers, Electric fields, *Multiphoton ionization, *Hydrogen atoms, *Photoionization, Laser radiation, Tunable lasers.

The photoionization of the H atom in strong electric fields, F , by resonant two-photon excitation, $H(1) + VUV \rightarrow H(2) + UV \rightarrow H(1) + e$, has been investigated at energies from the classical field ionization saddle point, $E(sp) = -2$ (the square root of F) a.u., through the zero field ionization limit, $E = 0$, into the continuum, $E > 0$. The atoms have been excited to single Stark levels in $n = 2$ with tunable pulsed VUV laser light around the Lyman-alpha line in an atomic beam with sub-Doppler resolution. The ionization from selected Stark levels by the UV was observed as a function of the UV wavelength.

500,306

PB85-221869

Not available NTIS
National Bureau of Standards, Gaithersburg, MD.

Role of Melting-Recrystallization Mechanism in Deformation of Crystalline Polymers.

Final rept.,

W. L. Wu, H. G. Zachmann, and C. Rickel. 1984, 3p

Pub. in Polym. Commun. 25, n3 p76-78 1984.

Keywords: *Synchrotron radiation, *Deformation methods, *Fibers, X ray stress analysis, Mechanical analysis, Melting, Recrystallization, Comparison, Reprints, *Small angle scattering, *Crystalline polymers.

Synchrotron radiation source at DESY, Hamburg, of West Germany, was used to carry out a small angle x-ray scattering (SAXS) study on the deformation mechanisms of oriented PET yarns. The stress-induced changes in the fiber morphology detected by SAXS can best be interpreted by a mechanical scheme instead of a melting-recrystallization mechanism.

500,307

PB85-221877

Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.

Studies of Microstructure in Native Celluloses Using Solid-State ¹³C NMR.

Final rept.,

D. L. Vanderhart, and R. H. Atalla. 1983, 9p

Sponsored by Technical Association of the Pulp and Paper Industry, Atlanta, GA.

Pub. in Proceedings of International Conference on Dissolving and Specialty Pulps, Boston, MA., April 5-8, 1983, p207-215.

Keywords: *Cellulose, *Microstructure, *Crystal structure, *Nuclear magnetic resonance, *Isotopic labeling, Polymorphism, Biochemistry.

High-resolution solid-state (^{13}C) NMR spectra have been taken on several native cellulosic materials as well as on a regenerated, low DP cellulose I material. Resonance multiplicities are observed for several carbon positions in the anhydroglucose units. The narrow-line multiplets, which are assigned to chains in the interior of crystallites, show significant variations in relative multiplet intensities, implying that native celluloses exhibit heterogeneous crystal structures. On the basis of these spectra it is proposed that all native celluloses are a mixture of two crystalline modifications, cellulose I(sub alpha) and I(sub beta). All native celluloses examined represent mixtures of these two structures in various proportions. There is no indication in the samples that each elementary fibril must contain the mixture of the two forms typical of the bulk sample. Therefore, the possibility that native celluloses are bio-synthetically-tailored composites certainly exists.

500,308

PB85-221893 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.

PSD and ESD (Photon and Electron Stimulated Desorption) of Condensed Films: Relevance to the Mechanism of Ion Formation and Desorption.

Final rept.,
R. Stockbauer, E. Bertel, and T. E. Madey. 1983, 2p
Pub. in Proceedings of International Workshop on Desorption Induced by Electronic Transitions (DIET I) (1st), Williamsburg, VA., May 12-14, 1982, p267-268 1983.

Keywords: *Thin films, *Water, *Methyl alcohol, *Cyclohexane, *Ionization, Desorption, Electron transitions, Chemical bonds, *Electron stimulated desorption, *Photon stimulated desorption, *Time of flight mass spectroscopy, Ion induced desorption.

Photon and electron stimulated desorption (PSD and ESD) have been used to study the electronic processes leading to ion formation in condensed films of water, methanol, and cyclohexane (C_6H_{12}). The dominant ions from condensed layers of water and methanol are $\text{H}^+(+1)$. Higher mass ions were less than 1% at all thicknesses. In contrast, heavy fragments $\text{C}_2\text{H}^+(\text{sub } n)$ - $\text{C}_5\text{H}^+(\text{sub } n)$ were observed for films of C_6H_{12} at doses above 10L . It is likely that heavy ions are effectively reneutralized in thin films of C_6H_{12} or by a de-excitation mechanism provided by hydrogen-bonding in the thick water and methanol films.

500,309

PB85-221901 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.

Validation of Analytical Methods.

Final rept.,
J. K. Taylor. 1983, 9p
Pub. in Analytical Chemistry 55, n6 pA600-A608 1983.

Keywords: *Chemical analysis, *Laboratory equipment, Standards, Quality assurance, Reprints, *Reference materials, Procedures.

Chemical measurements are made using procedures which operationally describe the methodology employed. A valid method is one which is capable of producing data of adequate quality for the intended use. Such methods are based upon sound principles established as the result of research and development endeavors of the scientific and technical community. Methods based on such validated measurement principles are developed and tested by individual scientists and are frequently reduced to practical procedures by standardization bodies. Such procedures should clearly describe both their utility and limitations. However, it remains the responsibility of each individual analyst to validate the applicability of every method and procedure used in each measurement situation, since he, alone, is responsible for the validity of his data. The use of reference materials, as available, is an excellent way to accomplish the above purpose, but other approaches are possible. The rationale behind all of the above is described and discussed.

500,310

PB85-221935 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.

Methanation Activity of W(110).

Final rept.,
T. J. Udovic, R. D. Kelley, and T. E. Madey. 1985, 6p
Sponsored by Department of Energy, Washington, DC. Office of Basic Energy Sciences.
Pub. in Surface Science 150, pL71-L76 1985.

Keywords: *Surface chemistry, *Catalysis, *Activation energy, Partial pressures, Temperature, Hydrogenation, Tungsten carbides, Reprints, *Methanation, Auger electron spectroscopy.

The methanation activity of W(110) was measured over a range of reactant partial pressures and temperatures ($P_{\text{sub H}_2} = 1\text{-}1000\text{ Torr}$, $P_{\text{sub CO}} = 0.1\text{-}10\text{ Torr}$, $T = 475\text{-}820\text{ K}$). Plotting the results in an Arrhenius fashion yielded a lower apparent activation energy ($E_{\text{sub a}} = 56\text{ kJ/mol}$) than previously determined for Ni(100) ($E_{\text{sub a}} = 103\text{ kJ/mol}$) with an activity surpassing that of Ni at lower temperatures. The H_2 pressure dependence of the methanation activity was found to be much stronger for W(110) than for Ni(100), the surface becoming increasingly inactive at the lowest H_2 pressures investigated. Auger electron spectroscopy revealed the active catalytic surface to be carbidic in nature.

500,311

PB85-221943 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.

Electron-Electron Interaction in Doubly-Excited States of Atoms.

Final rept.,
A. R. P. Rau. 1984, 7p
Pub. in Pramana 23, n3 p297-303 Sep 84.

Keywords: *Atomic energy levels, Excitation, Comparison, Quantum numbers, Ions, Angular momentum, Reprints, *Electron-electron collisions, *Isoelectronic sequence, *Hydrogen ions, Numerical analysis.

Doubly excited states of the isoelectronic sequence of $\text{H}(-1)$, in which both electrons are in high principal quantum numbers, are examined on the basis of alternative pictures of the correlations between the two electrons. Restricting ourselves to the lowest singlet S states with both electrons in principal quantum number n , the author parameterized the electron-electron interaction on the basis of these pictures and compare the resulting simple expressions with more elaborate numerical calculations. This provides further understanding of the nature of correlations in such states.

500,312

PB85-221976 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.

Unusual C-O Bond Weakening on a Clean Metal Surface: CO on Cr(110).

Final rept.,
N. D. Shinn, and T. E. Madey. 24 Dec 84, 4p
Sponsored by Department of Energy, Washington, DC., and National Research Council of Canada, Ottawa (Ontario).
Pub. in Physical Review Letters 53, n26 p2481-2484, 24 Dec 84.

Keywords: *Carbon monoxide, *Chemisorption, *Surface chemistry, *Chemical bonds, *Weak interactions, Chromium, Metals, Electron diffraction analysis, Spectroscopic analysis, Molecular structure, Reprints, *Molecular configuration, Electron energy loss spectroscopy, Auger electron spectroscopy, Electron stimulated desorption angular distributions, Low energy electron diffraction.

A unique CO chemisorption mode ($\alpha(\text{sub } 1)\text{CO}$), with the lowest reported CO stretching frequencies ($1150\text{-}1330\text{ cm}^{-1}$) on any clean or promoted metal surface, has been identified on Cr(110) using EELS, ESDIAD, LEED, AES, and oxygen coadsorption experiments. A 'lying down' binding configuration in two-fold symmetric hollow sites is proposed for ($\alpha(\text{sub } 1)\text{CO}$) molecules.

500,313

PB85-221992 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Chemical Thermodynamics Div.

Determination of Molecular Weight Distribution of Aromatic Components in Petroleum Products by Chemical Ionization Mass Spectrometry with Chlorobenzene as Reagent Gas.

Final rept.,
L. W. Sieck. 1983, 4p
Sponsored by Department of Energy, Washington, DC. Office of Basic Energy Sciences.

Pub. in Analytical Chemistry 55, n1 p38-41 1983.

Keywords: *Molecular weight, *Aromatic compounds, *Petroleum products, Fuels, Mass spectroscopy, Benzenes, Naphthalenes, Reprints, *Chemical ionization mass spectroscopy, *Chemical reaction mechanisms, *Charge exchange reactions, Benzene/chloro.

A chemical ionization mass spectrometric technique for direct determination of the molecular weight distributions of the major aromatic components in liquid fuels and other petro-products is discussed. The basic mechanism involves selective charge exchange reactions between chlorobenzene cations and the substituted benzenes and naphthalenes present in the sample. Chlorobenzene also serves as the solvent for the fuel, and screening of successive samples can be carried out with a 3-min turn-around time. Depending upon conditions, the paraffinic components present in the fuel are absent in the resulting mass spectrum.

500,314

PB85-222032 Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.

Laser Probing of Chemical Reaction Dynamics.

Final rept.,
S. R. Leone. 22 Feb 85, 7p
Contracts NSF-PHY82-00805, DAAG29-82-K-0031
Sponsored by Air Force Office of Scientific Research, Arlington, VA.
Pub. in Science 227, p889-895, 22 Feb 85.

Keywords: *Molecular energy levels, *Chemical reactivity, *Dynamics, Molecular vibration, Molecular rotation, Excitation, Electron transitions, Reprints, *Laser enhanced reactions, *Laser induced excitation, *Laser microprobe analysis.

Lasers are used in increasingly sophisticated ways to carry out reactions between molecules in selected vibrational, rotational, and electronic states and to probe the product states of chemical reactions. Such investigations are providing unprecedented insights into chemical reaction dynamics, which is the study of the detailed motions that molecules undergo in simple chemical reactions. In many cases it is possible to describe the influence that specific types of molecular excitation have on reactive events. Experiments are also being carried out to learn about chemical reactivity as a function of the alignment of reagents. There is increasing excitement concerning the potential of laser methods to interrogate the transition states of molecular reactions.

500,315

PB85-222057 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.

Determination of Molecular Structure at Surfaces Using Angle Resolved Electron and Photon-Stimulated Desorption.

Final rept.,
T. E. Madey, F. P. Netzer, J. E. Houston, D. M. Hanson, and R. Stockbauer. 1983, 19p
Contract DE-AC04-76DP00789
Sponsored by Office of Naval Research, Washington, DC.
Pub. in Proceedings of Int. Workshop Desorption Induced by Electronic Transitions (DIET I) (1st), Williamsburg, VA., May 12-14, 1982, p120-138 1983.

Keywords: *Molecular structure, *Surface chemistry, Chemisorption, Desorption, Comparison, Photons, Electron transitions, *Electron stimulated desorption ion angular distributions, *Proton stimulated desorption ion angular distributions.

The authors review recent data and theoretical models related to the use of angle-resolved electron and photon stimulated desorption in determining the structures of molecules at surfaces. Examples include a variety of structural assignments based on ESDIAD (electron stimulated desorption ion angular distributions), the observation of short-range local ordering effects induced in adsorbed molecules by surface impurities, the influence of electron-beam damage on surface structure, and a direct comparison of ESD and PSD ion yields for the same system.

500,316

PB85-222065 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymer Science and Standards Div.

Field 7—CHEMISTRY

Group 7D—Physical Chemistry

Concentration Dependence of the Diffusion and Permeability in a Homogeneous Membrane. 1. The Fickian and Chemical Potential Formulation of the Diffusion Current.

Final rept.,
A. Peterlin. 1985, 7p
Pub. in Colloid and Polymer Science 263, n1 p35-41 1985.

Keywords: *Membranes, *Sorption, *Permeability, *Polymeric films, *Diffusion coefficient, Concentration(Composition), Transport properties, Experimental design, Reprints, *Chemical potential, *Fick law.

For the sorption and diffusion coefficient dependence on the concentration of the penetrant the transport properties of a homogeneous medium are calculated. The diffusion current is assumed to be proportional to the negative gradient of the chemical potential. This is in contrast with the first Fick's law that assumes the current to be proportional to the negative gradient of the concentration of the penetrant. The difference between the two cases depends on the concentration dependence of the sorption coefficient. In a homogeneous membrane the chemical potential formulation leads to an equation which is very similar to the Fickian expression. The apparent diffusion coefficient, however, depends not only on the transport resistance but also on the deviation of the sorption coefficient from constancy.

500,317
PB85-222081 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymer Science and Standards Div.

Concentration Dependence of the Diffusion and Permeability in a Homogeneous Membrane. 2. The Differences between the Fickian and Chemical Potential Formulation in the Case of a Linear Increase of the Sorption Coefficient with the Equivalent Penetrant Pressure.

Final rept.,
A. Peterlin. 1985, 9p
Pub. in Colloid and Polymer Science 263, n1 p42-50 1985.

Keywords: *Membranes, *Sorption, *Permeability, *Polymeric films, *Diffusion coefficient, Concentration(Composition), Experimental design, Free energy, Pressure distribution, Reprints, *Chemical potential, *Fick law.

In a linear dependence of the sorption coefficient S on the equivalent pressure of the penetrant the differences between the Fickian and chemical potential formulation of the diffusion current are very soon larger than 20%, the assumed and tolerated error limit of the experiment. It turns out that the zero concentration diffusion coefficient $D(\text{sub } 0)$ determined from the sorption or permeation transient on the basis of the chemical potential basis is larger than that determined on the basis of Fick's law.

500,318
PB85-222099 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.

Adsorption of Oxygen on Ag(110): A New View of Structure and Bonding.

Final rept.,
K. Bange, T. E. Madey, and J. K. Sass. 4 Jan 85, 7p
Sponsored by Deutsche Forschungsgemeinschaft, Bonn-Bad Godesberg (Germany, F.R.).
Pub. in Chemical Physics Letters 113, n1 p56-62, 4 Jan 85.

Keywords: *Molecular structure, *Chemical bonds, *Oxygen, *Surface chemistry, Silver, Adsorption, Reprints, *Molecular configurations, *Electron stimulated desorption ion angular distributions.

The authors have used ESDIAD (electron stimulated desorption ion angular distributions) to characterize the structure and bonding of O₂ on Ag(110). Possible structures are discussed which are at variance with existing models of the oxygen-Ag(110) system.

500,319
PB85-222347 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.

Surface Tension of Liquid Silicon.

Final rept.,
S. C. Hardy. 1984, 5p
Sponsored by National Aeronautics and Space Administration, Washington, DC.

Pub. in Jnl. of Crystal Growth 69, p456-460 1984.

Keywords: *Silicon, *Interfacial tension, Liquids, Measurement, Impurities, Reprints, Temperature dependence.

The surface tension of liquid silicon has been measured as a function of temperature in purified argon atmospheres using the sessile drop technique. The measurements show the surface tension is sensitive to low levels of an impurity which is probably oxygen. The highest surface tension values obtained under conditions which minimized the oxygen levels in the apparatus are in good agreement with an isolated previous measurement in pure hydrogen. The surface tension decreases linearly with increasing temperature and has a temperature coefficient of $-0.28 \text{ mJ/(m squared)K}$.

500,320
PB85-222370 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.

Trajectory Approach to the Hydrogen Evolution Reaction.

Final rept.,
S. Holloway, and J. W. Gadzuk. 1983, 6p
Pub. in Nordic Conf. on Surface Science, Tampere, Finland, August 18-20, 1982, Physica Scripta T4, p86-91 1983.

Keywords: *Hydrogen, *Electrochemistry, *Dynamics, Surface chemistry, Equations of motion, Potential energy, Reaction kinetics, Chemical reactions, Solvents.

A classical trajectory analysis for the discharge reaction step in the hydrogen evolution reaction is presented. The construction of an adiabatic potential energy surface is discussed with emphasis on the solvent motion and the charge transfer process. Corrections to absolute rate theory reaction probabilities arising from dynamical effects are presented as a function of applied potential.

500,321
PB85-222396 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Molecular Spectroscopy Div.

Infrared Multiphoton Dissociation of Methyl Nitrite in a Molecular Beam: Internal States of the Nitric Oxide Fragment.

Final rept.,
D. S. King, and J. C. Stephenson. 1 Mar 85, 4p
Sponsored by Army Research Office, Arlington, VA., and Office of Naval Research, Arlington, VA.
Pub. in Jnl. of Chemical Physics 82, n5 p2236-2239, 1 Mar 85.

Keywords: *Nitrogen oxide(NO), *Dissociation, *Spectroscopic analysis, *Pulse transmission, *Molecular beams, Molecular rotation, Molecular energy levels, Excitation, Spin orbit interactions, Reprints, *Laser excited fluorescence, *Laser spectroscopy, *Methyl nitrite, *Rotational energy levels.

The rotational-, spin-, and lambda doublet-state distributions for nitric oxide (NO) formed in the CO₂ laser multiphoton dissociation of methyl nitrite, CH₃ONO, in a pulsed molecular beam are reported. There is no apparent preference for formation of either lambda doublet component and there is no observable fragment alignment, the nascent NO species exhibiting an isotropic distribution of angular momentum vectors.

500,322
PB85-222404 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Molecular Spectroscopy Div.

Kinetic Energy Disposal in the Unimolecular IRMPD of Methyl Nitrite in a Pulsed Molecular Beam.

Final rept.,
D. S. King, and J. C. Stephenson. 15 Mar 85, 6p
Sponsored by Army Research Office, Arlington, VA., and Office of Naval Research, Arlington, VA.
Pub. in Chemical Physics Letters 114, n5-6, p461-466, 15 Mar 85.

Keywords: *Kinetic energy, *Dissociation, *Spectroscopic analysis, *Molecular beams, *Pulse transmission, Molecular rotation, Molecular energy levels, Excitation, Spin orbit interactions, Doppler effects, Temperature, Nitrogen oxide(NO), Reprints, *Laser excited fluorescence, *Methyl nitrite, *Laser spectroscopy, *Rotational energy levels.

Methyl nitrite, CH₃ONO, was dissociated by infrared laser pulses of well defined intensity under collisionless conditions in a pulsed molecular beam. Doppler-resolved laser-excited fluorescence spectroscopy determined the kinetic energy of the nitric oxide fragments formed in particular quantum states. The observed Doppler profiles were Gaussian over two e-foldings and, when converted to translational temperatures, corresponded to temperatures in the range of 260 to 350 K for states with 40 to 1308/cm of rotational energy; no significant correlation was observed between rotational, spin-orbit, or lambda doublet/state and kinetic energy.

500,323
PB85-225225 PC A03/MF A01
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.
Model Describing the Steady-State Pyrolysis of Bubble-Forming Polymers in Response to an Incident Heat Flux,
I. S. Wichman. May 85, 48p NBSIR-85/3130

Keywords: *Mathematical models, *Bubbles, *Thermoplastic resins, *Heat flux, *Gasification, Steady state, Heat transmission, Transport properties, Nucleation, Equations of state, Surface chemistry, Mass transfer, *Chemical reaction mechanisms, Monomers.

A theoretical model is developed to describe the in-depth effect of bubbles on the steady-state transport of volatile gases (monomer) from the surface of a polymer subjected to an incident heat flux. In this model the effect of the bubbles on the surrounding (liquid) polymer is felt through the bubble number distribution function, n , which appears in the equations for conservation of mass, momentum, species and energy in the melt. The equation for the evolution of n includes the effects of bubble growth, convection and nucleation; its derivation requires preliminary study of the growth and motion of an individual bubble in a liquid with a temperature gradient. With these equations, formulas for the mass flux of volatiles from the polymer surface and the bubble void fraction are developed, for the special case of constant polymer mass fraction.

500,324
PB85-225688 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Organic Analytical Research Div.

Determination of Nitro-Polynuclear Aromatic Hydrocarbons in Diesel Soot by Liquid Chromatography with Fluorescence and Electrochemical Detection.

Final rept.,
W. A. MacCrehan, and W. E. May. 1985, 12p
Pub. in Proceedings of Int. Symp. Polynuclear Aromatic Hydrocarbons: Mechanisms, Methods, and Metabolism (8th), p857-869 1985.

Keywords: *Aromatic polycyclic hydrocarbons, *Exhaust emissions, *Fluorescence, *Electrochemistry, *Nitroaryl compounds, *Chemical analysis, *Soot, Distillation, Sampling, Air pollution, *Air pollution detection, *High performance liquid chromatography, *Diesel engine exhaust.

Two new detection approaches for the HPLC determination of nitro-polynuclear aromatic hydrocarbons (N-PAH) are described. The molecular fluorescence method is based on the reduction of the nitro group to the fluorescent amine using a post-column zinc reductor. Wavelength programming is used to improve the selectivity and sensitivity of the detection of N-PAH. The electrochemical detection method uses the reduction current of the nitro group for measurement of the N-PAH. A differential pulse waveform is used to enhance the selectivity of the detector. Sample preparation methods for N-PAH in diesel soot are described.

500,325
PB85-225696 Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.

Saturation of Continuum-Continuum Transitions in Multiphoton Absorption.

Final rept.,
K. Rzazewski, and R. Grobe. 15 Apr 85, 1p
Pub. in Physical Review Letters 54, n15 1729p, 15 Apr 85.

Keywords: *Continuum mechanics, *Mathematical models, Dipole moments, Atomic theory, Reprints, *Hydrogen atoms.

The author comment on a recent letter by Deng and Eberly (Phys. Rev. Lett. 53, 1810 (1984)) and suggest a specific experiment which could test the model developed by those authors.

500,326

PB85-225704 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Atomic and Plasma Radiation Div.

Resonant Transitions of Kr X.

Final rept.,
J. Reader, A. N. Ryabtsev, and A. A. Ramonas. Mar 85, 5p
Sponsored by Department of Energy, Washington, DC.
Pub. in Jnl. of the Optical Society of America B 2, n3 p417-421 Mar 85.

Keywords: *Krypton, *Spectroscopic analysis, *Line spectra, Hartree-Fock approximation, Least squares method, Reprints, *Krypton ions.

The spectrum of nine-times ionized krypton, KrX, was observed with a low-inductance vacuum spark and a 10.7-m grazing-incidence spectrograph. Forty-four spectral lines in the region 91-105 Å were classified. The identifications were made with the aid of Hartree-Fock and least-squares parametric calculations.

500,327

PB85-225720 Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.

Collisions in the Presence of a Laser Field and the Laser as a Tool for State Selective Preparation of Molecular States in Collisions.

Final rept.,
I. V. Hertel. Jan 85, 5p
Pub. in Jnl. de Physique 46, n1 pCL37-CL41 Jan 85.

Keywords: *Molecular energy levels, Excitation, Ions, Laser beams, Atoms, Reprints, *Laser spectroscopy, *Laser induced excitation, *Molecule-molecule collisions, Ion-atom collisions.

In the study of individual collision events laser light can be used to influence or probe the process prior to, during, or after the binary particle interaction. The author discusses some problems and particularly challenging possibilities for modifying the collision process in a high, but not too high, laser field. He discusses the possibilities of state selective preparation of quasimolecular sigma and pi states in ion-atom collisions, with asymptotically laser optical pumped atomic p-states.

500,328

PB85-225738 Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.

Anisotropic Scattering of Electrons by N₂ and Its Effect on Electron Transport.

Final rept.,
A. V. Phelps, and L. C. Pitchford. May 85, 18p
Grant ARO-8-82
Pub. in Physical Review A 31, n5 p2932-2949 May 85.

Keywords: *Electron transfer, *Electron scattering, *Nitrogen, *Anisotropy, Transport properties, Spatial distribution, Ionization, Excitation, Mathematical models, Elastic scattering, Experimental design, Boltzmann equation, Inelastic scattering, Reprints, *Electron-molecule collisions.

As part of a systematic study of approximations commonly made in solutions of the Boltzmann equation for electrons in molecular gases, the authors have investigated the effects of anisotropic scattering on electron transport coefficients in N₂ and have extended our study of the multiterm expansion technique to higher E/n. The importance of proper interpretation of ionization and excitation experiments at high E/n is illustrated by calculations which model either an exponential growth of density in time or an exponential growth with position. The calculated excitation coefficients are generally higher than experiment at low and high E/n but in agreement with experiment at E/n near 150 Td.

500,329

PB85-225746 Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.

Absolute Cross-Section Measurements for Electron-Impact Ionization of Doubly Charged Ions Ti(+2), Fe(+2), Ar(+2), Cl(+2) and F(+2).

Final rept.,
D. W. Mueller, T. J. Morgan, G. H. Dunn, D. C. Gregory, and D. H. Crandall. May 85, 9p
Contract DOE-EA-77-A-0101
Pub. in Physical Review A 31, n5 p2905-2913 May 85.

Keywords: *Ionization coefficients, *Reaction kinetics, *Collision cross sections, Temperature, Excitation, Comparison, Reprints, *Electron-ion collisions, *Autoionization, Numerical solution, Iron ions, Chloride ions, Fluoride ions, Argon ions, Titanium ions.

Measurements have been made of the cross section for electron-impact single ionization of the ions Ti(+2), Fe(+2), Ar(+2), Cl(+2), and F(+2), spanning the range of energies from below threshold to 1500 eV. Indirect processes such as excitation-autoionization contribute substantially to the cross section for Ti(+2), while such contributions are less pronounced for the other species. Comparisons with available theoretical predictions and with the Lotz semiempirical formula are presented. Expansion coefficients and formulas for generating ionization rate coefficients in the temperature range 10,000 < T < 10,000,000 K are included for each ion.

500,330

PB85-226033 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Chemical Kinetics Div.

Structures of C₆H₇(+1) Ions Formed in Unimolecular and Bimolecular Reactions.

Final rept.,
S. G. Lias, and P. Ausloos. 15 Apr 85, 12p
Sponsored by Air Force Office of Scientific Research, Bolling AFB, DC.
Pub. in Jnl. of Chemical Physics 82, n8 p3613-3624, 15 Apr 85.

Keywords: *Molecular structure, *Reaction kinetics, *Isomerization, *Spectroscopic analysis, Stereochemistry, Heats of formation, Benzenes, Molecular energy levels, Mass spectroscopy, Cyclohexadiene compounds, Reprints, *Benzenium ions, *Chemical reaction mechanisms, *Fragmentation patterns(Mass spectroscopy), *Proton affinity, *Photoisomerization, Ion cyclotron resonance mass spectroscopy, Hexatriene, Cyclohexadiene.

The structures, isomerization mechanisms, and reaction kinetics of C₆H₇+7 ions formed in a variety of systems have been studied. The ions formed in the reactions (H₂C=C=CH₂(+1)+H₂C=C=CH₂) and (HC=CCH₃(+1)+HC=CCH₃) as well as the fragment C₆H₇(+1) ions in 1,3-cyclohexadiene, 1,4-cyclohexadiene, trans-1,3,5-hexatriene, 1-methylcyclopentene, 3-methylcyclopentene, and 4-methylcyclopentene exhibit at least two structures under the conditions of an ICR experiment. In each case, one isomer transfer a proton to bases with proton affinity higher than that of benzene demonstrating that the species has the benzenium (protonated benzene) structure. The energetics of the fragmentation process leading to C₆H₇(+1) formation have been examined in a photoelectron-photoion coincidence spectrometer for trans-1,3,5-hexatriene and 1,3- and 1,4-cyclohexadiene. It is found that the transition state for the fragmentation process (C₆H₈(+1) yields C₆H₇(+1)+H) is effectively the same in all three systems but lies at an energy level higher than (benzenium ion +H) products. Rate constants for reactions of benzenium ions with a variety of organic and inorganic compounds have been determined.

500,331

PB85-226041 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Atomic and Plasma Radiation Div.

Resonance Transitions 4d(sup 10)5s - 4d(sup 9)5s5p In the Ag I Sequence of In III, Sn IV, Sb V, and Te VI.

Final rept.,
V. Kaufman, J. Sugar, T. A. M. van Kleef, and Y. Joshi. Mar 85, 4p
Pub. in Jnl. of the Optical Society of America B 2, n3 p426-429 Mar 85.

Keywords: *Molecular energy levels, *Ions, *Eigenvalues, Antimony, Cadmium, Indium, Tellurium, Tin, Wavelengths, Reprints, *Isoelectronic sequence, *Molecular configuration, Resonant transfer.

Nearly complete resonance transition arrays 4d (sup 10)5s-4d (sup 9)5s5p in the Ag I isoelectronic se-

quence were observed in sliding and triggered sparks for the ions In III through Te VI. Wavelengths and estimated relative intensities are given as well as energy levels and eigenvectors for the upper levels. Evidence of configuration interaction is indicated by the irregular behavior of the fitted radial energy integrals for 4d (sup 9)5s5p, but no attempt was made to add configuration interaction.

500,332

PB85-226066 PC A03/MF A01
National Bureau of Standards (NML), Boulder, CO. Chemical Engineering Science Div.

Experimental Thermal Conductivity Values for Mixtures of Methane and Ethane.

Final rept.,
H. M. Roder, and D. G. Friend. Mar 85, 43p NBSIR-85/3024

Keywords: *Methane, *Ethane, *Thermal conductivity, Mixtures, Experimental design, Pressures, Temperatures, Density(Mass/volume), Tables(Data).

The experimental measurements of thermal conductivity as obtained in a transient hot wire apparatus for mixtures of methane and ethane are recorded. The measurements were made at temperatures between 140 and 330 K with pressures between 0.1 and 70 MPa. The density range is 0 to 24 mol/L, the mole fractions of methane are 0.69, 0.50, and 0.35, and the total number of points recorded is 2476.

500,333

PB85-227072 PC A06/MF A01
National Bureau of Standards (NML), Gaithersburg, MD. Center for Radiation Research.

Bibliography on Atomic Energy Levels and Spectra, July 1979 through December 1983.

Interim rept.,
A. Musgrove, and R. Zalubas. Jun 85, 124p NBS/SP-363-SUPPL-3
See also PB81-125833. Also available from Supt. of Docs as SN003-003-02661-1. Library of Congress catalog card no. 85-600543.

Keywords: *Atomic energy levels, *Atomic spectra, *Bibliographies, Atoms, Ions, Spectral lines, Wavelengths, Zeeman effect, Hyperfine structure, Ionization potentials, Isotope effect, Tables(Data).

This is the third supplement to NBS Special Publication 363. Bibliography on Atomic Energy Levels and Spectra, July 1968 through June 1971. Supplement 1 covered the period from July 1971 through June 1975, Supplement 2 covered the period from July 1975 through June 1979, and this bibliography covers the literature from July 1979 through December 1983. It contains approximately 1200 references classified by subject for individual atoms and atomic ions. A number index identifies the references. An author index is included. References included contain data on energy levels, classified lines, wavelengths, Zeeman effect, Stark effect, hyperfine structure, isotope shift, ionization potentials, or theory which gives results for specific atoms or atomic ions.

500,334

PB85-227569 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Atomic and Plasma Radiation Div.

Discrete 4D Photoabsorption Spectrum of Ba(+2).

Final rept.,
C. W. Clark. Aug 84, 5p
Sponsored by National Research Council, Washington, DC., and Air Force Office of Scientific Research, Bolling AFB, DC.
Pub. in Jnl. of the Optical Society of America B 1, n4 p626-630 Aug 84.

Keywords: *Absorption spectra, Far ultraviolet radiation, Ultraviolet spectra, Reprints, *Barium ions.

The role of true collective effects in the 4d photoabsorption spectrum of Ba(+2) is shown to be minor. The most significant departures from independent particle behavior are in fact due to correlations involving the 5p, not the 4d, shell; their importance is magnified by the delicate balance of opposing single-particle forces. Reevaluation of the ionization limit reveals the presence of Beutler-Fano structures in the experimental data, the first that have been observed for excitations underneath closed shells.

Field 7—CHEMISTRY

Group 7D—Physical Chemistry

500,335

PB85-227577 Not available NTIS
National Bureau of Standards (NML), Boulder, CO.
Quantum Physics Div.

Detection of Nitrogen Rotational Distributions by Resonant 2 + 2 Multiphoton Ionization Through the $a(\text{sup } 1)\pi(\text{sub } g)$ State.

Final rept.,
K. L. Carleton, K. H. Welge, and S. R. Leone. Apr 85, 4p
Contract DE-AC02-79ER10396, Grant NSF-CHE79-11340
Sponsored in part by Grant NSF-PHY82-00805.
Pub. in Chemical Physics Letters 115, n6 p492-495, 19 Apr 85.

Keywords: *Molecular rotation, *Nitrogen, *Ionization, Photons, Reprints, *Laser induced ionization, *Rotational energy levels.

Characterization of laser 2+2 multiphoton ionization of nitrogen to obtain rotational state distributions has been investigated via the resonant two-photon transition. For room-temperature nitrogen, the spectral intensities and state distribution are directly related and give rotational temperatures of 290 ± 20 K. For power densities of 3 GW/sq cm, the ionization probability is .00001 per N₂ molecule per average rotational state.

500,336

PB85-227585 Not available NTIS
National Bureau of Standards (NML), Boulder, CO.
Quantum Physics Div.

Collisional Redistribution of Circularly Polarized Light in Barium Perturbed by Argon.

Final rept.,
W. J. Alford, N. Andersen, M. Belsley, J. Cooper, and D. M. Warrington. May 85, 5p
Grant NSF-PHY82-00805
Pub. in Physical Review A 31, n5 p3012-3016 May 85.

Keywords: *Barium, *Molecular energy levels, *Molecular orbitals, Circular polarization, Excitation, Molecular orbitals, Pressure, Reprints, *Molecule-molecule collisions, Polarized light.

The authors have measured the orientation of the Ba 6p¹P level produced by collision-induced excitation from the ground state by circularly polarized light. The detuning dependence of the far-wing excited-state orientation can be interpreted in terms of reorientation of molecular orbitals which occur during the collision. Effects due to rotational coupling are seen to occur at large blue-wing detunings. They have also determined the collisional rate for destruction of orientation by measuring the pressure dependence of the excited-state orientation.

500,337

PB85-227593 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Organic Analytical Research Div.

Determination of Dibenzothiophene in Oils by Liquid Chromatography-Tandem Mass Spectrometry.

R. G. Christensen, and E. White. 1985, 4p
Pub. in Jnl. of Chromatography 323, p33-36 1985.

Keywords: *Trace elements, *Chemical analysis, *Fuel oil, *Crude oil, Chromatographic analysis, Mass spectroscopy, Sampling, Reprints, *Liquid chromatography, *Dibenzothiophene.

Quantitative trace analysis for organic compounds in complex matrices such as oils often requires time-consuming sample pretreatment. Two examples are shown of the use of a highly selective tandem mass spectrometer as a liquid chromatographic detector for the quantification of dibenzothiophene in a crude petroleum oil and in an alternate fuel oil. No sample preparation except an appropriate dilution was required. A preconcentrating liquid chromatography-mass spectrometry interface was used, allowing detection limits of ca. 20 microgram to be attained.

500,338

PB85-227601 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.

Angle-Resolved Photoelectron Study of the Valence Levels of BF₃ in the Range $17 = h(\nu) = 28\text{eV}$.

Final rept.,
J. L. Dehmer, A. C. Parr, S. H. Southworth, and D. M. P. Holland. Oct 84, 8p
Grant NATO-1939
Sponsored by Department of Energy, Washington, DC., and Office of Naval Research, Arlington, VA.
Pub. in Physical Review A 30, n4 p1783-1790 Oct 84.

Keywords: *Photochemical reactions, *Ionization, *Boron fluorides, *Molecular energy levels, *Photoelectric emission, Mathematical models, Experimental design, Comparison, Angular distribution, Reprints.

Photoelectron branching ratios and angular distributions have been measured for the six outermost levels of BF₃ in the range $17 < \text{or} = h\nu < \text{or} = 28$ eV with the use of synchrotron radiation. Comparisons are made with a recent multiple-scattering model calculation which indicates that a shape resonance in the e⁻ electronic continuum should appear in five of the six channels studied. Good agreement between experiment and theory is found in a majority of the comparisons; however, experimental evidence for the expected e⁻ shape resonance is clear in some cases but absent in others. The results are discussed in the context of other cases in which shape resonances, well known from inner-shell spectra, are obscured in valence-shell properties. Experiments which would help clarify the role of the e⁻ shape resonance in the photoionization dynamics of BF₃ are suggested.

500,339

PB85-227619 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.

Multiple-Pulse Proton NMR of Pressure-Crystallized Linear Polyethylene.

Final rept.,
J. R. Havens, and D. L. VanderHart. 1985, 3p
Pub. in Jnl. of Magnetic Resonance 61, p389-391 1985.

Keywords: *Nuclear magnetic resonance, *Polyethylene, Molecular relaxation, Crystallization, Anisotropy, Pressure, Reprints, *Chemical shift(Nuclear magnetic resonance).

The multiple-pulse proton NMR spectrum of pressure-crystallized linear polyethylene is reported. A clearly defined axially symmetric chemical shift tensor is observed, whose anisotropy has a width of approximately 6.9 ppm. Use of a spherical sample is seen to reduce broadening from bulk magnetic susceptibility effects. A comparison of the effectiveness of two multiple-pulse sequences is made based on the linewidths. Relaxation behavior under multiple pulse is also reported and leads to an estimate of the percentage crystallinity of this sample in excess of 90%.

500,340

PB85-227627 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Thermophysics Div.

Molecular Dynamics Study of the Liquid and Plastic Phases of Neopentane.

Final rept.,
R. D. Mountain, and A. C. Brown. May 85, 7p
Pub. in Jnl. of Chemical Physics 82, n9 p4236-4242 May 85.

Keywords: *Phase transformation, *Liquid phases, Molecular rotation, Plasticity, Reprints, *Molecular dynamics, *Propane/dimethyl, Molecular models.

Molecular dynamics has been used to investigate a model for neopentane. The velocity-velocity and angular momentum-angular momentum time correlation functions were constructed for the liquid and the single particle time correlation functions for the orientation of twofold and threefold axes of symmetry of the molecules were constructed for both the liquid and plastic phases. The model produces liquid properties that are in agreement with those of liquid neopentane. The dynamics of the molecular reorientations in the plastic phase has been examined. These reorientations are found to consist of jumps between equivalent orientations by a rotation of 120 degrees around a threefold molecular symmetry axis.

500,341

PB85-227684 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.

NMR (Nuclear Magnetic Resonance) Self-Diffusion Study of Polyethylene and Paraffin Melts.

Final rept.,
I. Zupancic, G. Lahajnar, R. Blinc, D. H. Reneker, and D. L. Vanderhart. 1985, 18p
Pub. in Jnl. of Polymer Science, Polymer Physics Edition 23, p387-404 1985.

Keywords: *Nuclear magnetic resonance, *Polyethylene, *Diffusion coefficient, *Alkanes, *Melts, Molecular weight, Transport properties, Reprints.

The self-diffusion coefficient D of paraffin and polyethylene melts—covering the range between N = 19 and 1,000 where N is the number of monomeric units—was measured by the pulsed-magnetic-field-gradient NMR method for diffusion times between 3 ms and 1 s. For the paraffins, D is proportional to 1/sq N though the molecular weights are smaller than the critical molecular weight for entanglement. In polyethylene, melts a strong dependence of the diffusion coefficient on the diffusion time is observed, whereas no such dependence is found in paraffin melts. A mathematical formalism for describing spin-echo attenuation in terms of a velocity autocorrelation function is shown to yield qualitative agreement with the experimental results.

500,342

PB85-228401 PC A03/MF A01
National Bureau of Standards (NML), Gaithersburg, MD. Center for Chemical Physics.

Bibliography of Sources of Thermodynamic Data for the Systems: CO₂+NH₃+H₂O, CO₂+H₂S+H₂O, H₂S+NH₃+H₂O, and CO₂+NH₃+H₂S+H₂O.

Final rept.,
R. N. Goldberg, and D. K. Steckler. May 85, 41p
NBS/SP-699
Also available from Supt. of Docs as SN003-003-02664-6. Library of Congress catalog card no. 85-600545. Sponsored by American Inst. of Chemical Engineers, New York.

Keywords: *Thermodynamic properties, *Bibliographies, *Chemical equilibrium, Thermodynamic equilibrium, Physical properties, Sources, Experimental design, Density(Mass/volume), Enthalpy, Sources, Tables(Data), Ammonium carbonate, Specific heat, Hydrogen sulfide, Carbon dioxide, Ammonia, Urea, Water.

Contained herein is a bibliography of sources of experimental and correlated thermodynamic data for the systems CO₂ + NH₃ + H₂O, CO₂ + H₂S + H₂O, H₂S + NH₃ + H₂O, and CO₂ + NH₃ + H₂S + H₂O. The types of data in this bibliography include all types of equilibrium data, including both equilibria in solution and vapor-liquid equilibrium data, enthalpies, heat capacities, and densities. There are 215 references cited.

500,343

PB85-229276 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Organic Analytical Research Div.

Separation and Purification of Diastereomers of Angiotensin I by Weak Anion-Exchange High-Performance Liquid Chromatography.

Final rept.,
S. A. Margolis, and M. Dizdaroğlu. 1985, 13p
Pub. in Jnl. of Chromatography 322, p117-128 1985.

Keywords: *Anion exchanging, *Purification, *Separation, *Chromatographic analysis, *Stereochemistry, Peptides, Separation, Comparison, Assessments, Reprints, *High performance liquid chromatography, *Angiotensin.

Several diastereomers of angiotensin I were resolved by weak anion-exchange high-performance liquid chromatography (HPLC). All of the diastereomers which were examined contained significant amounts of peptides whose amino acid composition differed from the designated diastereomer of angiotensin I. The results are compared with the results of separations of the same peptides by reversed-phase HPLC. The comparison strongly suggests that the two HPLC methods, utilizing different separation principles, are complementary; hence their combined use leads to a more confident assessment of the purity of a given peptide preparation.

500,344

PB85-229292 Not available NTIS

National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.

Excited Electron Correlations in Resonant Multiphoton Ionization via Barium Rydberg States.

Final rept.,
G. Leuchs, and S. J. Smith. 1985, 9p
Grant NSF-PHY82-00805
Pub. in Physical Review A 31, n4 p2283-2290 Apr 85.

Keywords: *Barium, *Angular distributions, *Photoionization, *Molecular energy levels, Excitation, Reprints, *Rydberg series, *Molecular configuration.

Photoelectron angular distributions have been studied in resonant multiphoton ionization of barium via $J=0$ states, in the region where the 6sns singlet $S(\text{sub } 0)$ Rydberg series interacts strongly with the 5d 7(triplet d)PO doubly excited state. The interaction is dominantly quadrupole and is localized around $n=18$. The data analysis reveals spin-orbit coupling and strong channel mixing in the continuum.

500,345
PB85-229326 Not available NTIS

National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.

Laser-Induced Fluorescence Measurement of Nascent Vibrational and Rotational Product State Distributions in the Charge Transfer of $\text{Ar}(+1) + \text{N}_2$ yields $\text{Ar} + \text{N}_2(+1)$ ($\nu=0,1$) at 0.2 eV.

Final rept.,
L. Huwel, D. R. Guyer, G. H. Lin, and S. R. Leone. 1984, 17p
Grants NSF-PHY82-00805, NSF-CHE79-11340
Sponsored by Air Force Office of Scientific Research, Bolling AFB, DC., and Petroleum Research Fund, Washington, DC.
Pub. in Jnl. of Chemical Physics 81, n8 p3520-3535 1984.

Keywords: *Reaction kinetics, *Fluorescence, *Supersonic nozzles, *Ionization chambers, Rotational vibration, Ions, Diatomic molecule, Reprints, *Laser induced fluorescence, *Ion molecule collision, Laser applications.

A novel experimental technique couples a flowing afterglow ion source with a supersonic nozzle expansion in order to deliver high densities of relatively low kinetic energy ions into a low pressure chamber. The technique is used to study the charge transfer reaction under single collision conditions at 0.24 eV c.m. Nascent rotational and vibrational state distributions are obtained by the method of saturated laser-induced fluorescence probing. It is found that a substantial fraction of the available energy is partitioned into internal excitation of the $\text{N}_2(+1)$ product molecule. The results are compared with a number of recent state-selected experiments on charge exchange in $\text{ArN}_2(+1)$, $\text{ArH}_2(+1)$ and $\text{NCO} (+1)$ systems. It is suggested the experimental findings are best explained in terms of the detailed locations of potential surface crossing seams, rather than by the widely used energy resonance or diatomic molecule, Franck-Condon ionization models.

500,346
PB85-229334 Not available NTIS

National Bureau of Standards, Gaithersburg, MD. Polymers Div.

Fluorescence Measurement of the Diffusion Coefficient for Butylated Hydroxyanisole in Low-Density Polyethylene.

Final rept.,
B. F. Howell, F. L. McCrackin, and F. W. Wang. 1985, 5p
Pub. in Polymer 26, p433-436 Mar 85.

Keywords: *Diffusion coefficients, *Antioxidants, *Fluorescence, Extraction, Reprints, *Low density polyethylene, *Phenol/butyl-hydroxy, *Cresol/dibutyl.

Measurement of the diffusion coefficient (D) of butylated hydroxyanisole (BHA) in low density polyethylene at 31°C was made by two techniques (1) Measurement of diffusion rate in the absence of solvent was made by use of a film stack with BHA-loaded discs on top and bottom. After a given diffusion time, the films were separated and the BHA extracted from the films into 1-propanol. (2) Fluorescence monitoring, under oxygen free conditions, was used to measure rate of BHA extraction from a film into 1-propanol at 31°C.

500,347
PB85-229342 Not available NTIS

National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.

Intensity-Dependent Electron Angular Distributions in Resonant Multiphoton Ionization.

Final rept.,
S. Geltman, and G. Leuchs. Mar 85, 8p
Grant NSF-PHY82-00805
Pub. in Physical Review A 31, n3 p1463-1469 Mar 85.

Keywords: *Angular distributions, *Photoionization, Hyperfine structure, Comparison, Experimental design, Ionization, Stark effect, Atomic energy levels, Anisotropy, Resonant frequency, Sodium, Reprints, *Sodium atoms.

A theoretical investigation has been carried out on the dependence of the photoelectron angular distributions on laser intensity for the case of two-photon-resonant three-photon ionization of sodium. Good overall agreement is obtained with the experimental anisotropy parameters for ionization via the $4D(3/2)$ and $4D(5/2)$ intermediate states. The comparison of the theoretical results with the experimental data also clearly shows that the hyperfine splitting of the ground state has to be taken into account at high laser intensities although the low intensity angular distributions do not depend on the initial ground hyperfine state.

500,348
PB85-229367 Not available NTIS

National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.

Resonance Scattering of a Short Laser Pulse on a Two-Level System: Time-Dependent Approach.

Final rept.,
M. Florjanczyk, K. Rzażewski, and J. Zakrzewski. Mar 85, 6p
Sponsored by National Aeronautics and Space Administration, Washington, DC.
Pub. in Physical Review A 31, n3 p1558-1562 Mar 85.

Keywords: *Resonance scattering, *Spectroscopic analysis, Fluorescence, Time dependence, Reprints, *Laser spectroscopy, *Laser induced fluorescence.

The authors discuss the time-dependent power spectrum of fluorescence light produced by a two-level system driven by a smooth, short, resonant laser pulse. They show how the multipeak structure of the spectrum develops in time. The possibility of a smooth transition to the conventional Mollow spectrum is discussed.

500,349
PB85-229383 Not available NTIS

National Bureau of Standards, Gaithersburg, MD. Polymers Div.

Infrared Bandshapes of Methylene-d₂ Bending Vibrations in n-Hexatriacontane-n-Hexatriacontane-d₇₄.

Final rept.,
B. Fanconi, F. McCrackin, and D. Sarazin. 1985, 11p
Pub. in Polymer 26, p219-228 Feb 85.

Keywords: *Infrared spectroscopy, *Deuterium compounds, *Band spectra, *Methylene, Isotopic labeling, Lattice parameters, Alkanes, Experimental design, Concentration(Composition), Reprints, *Hexatriacontane, Numerical solution.

Infra-red spectra in the CD₂ bending vibration region (1080-1100/cm⁻¹) have been analyzed for mixtures of deuterated and hydrogenated hexatriacontane. The i.r. data analyses are based on lattice dynamical calculations of guest deuterated molecules in the host n-C₃₆H₇₄ and infrared intensities calculated using the electro-optical parameter method. The calculated band profiles as a function of the deuterated molecule concentration compare favorably to experimental spectra taken at 80K. The high resolution, low temperature spectra reveal features heretofore only observed at much higher concentrations of deuterated species. Self deconvolution procedures were used to further resolve the spectra. Excellent agreement was found between calculated and experimental ratios of the i.r. intensity of certain dimer arrangements to that of singlet molecules. The intensity ratio was found to be a better measure of deuterated species concentration than the halfwidth of the CD₂ bending vibration band that had been previously used.

500,350
PB85-229409 Not available NTIS

National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.

Dielectronic Recombination.

Final rept.,
G. H. Dunn, D. S. Belic, N. Djuric, and D. W. Mueller. 1984, 19p
Pub. in Proceedings of the International Conference on Atomic Physics (9th), Seattle, Washington, July 1984, p505-522.

Keywords: Experimental design, Reviews, Cross sections, *Dielectronic recombination.

Within the past one and a half years, the process known as dielectronic recombination has for the first time been observed and measured in isolation from other processes. The measurements and comparison with theory have highlighted interesting physical phenomena as well as raised questions about the completeness of accepted theoretical treatments of the process.

500,351
PB85-229433 Not available NTIS

National Bureau of Standards, Gaithersburg, MD. Polymers Div.

Poly(ethylene imine)-Sodium Iodide Complexes.

Final rept.,
C. K. Chiang, G. T. Davis, C. A. Harding, and T. Takahashi. 1985, 4p
Sponsored by Office of Naval Research, Arlington, VA.
Pub. in Macromolecules 18, n4 p825-827 1985.

Keywords: *Complex compounds, *Differential thermal analysis, Inorganic salts, Concentration(Composition), Electrical resistance, Reprints, *Poly(ethylene imine), Monomers.

Sodium iodide can be incorporated into linear poly(ethylene imine) up to 0.3 moles of NaI per mole of monomer repeat. At low concentrations, the incorporation of salt inhibits the normal crystallization of the polymer while at high concentrations the salt and polymer form a complex crystal phase which melts near 150°C. The addition of NaI to the polymer initially increases d-c conductivity but the incorporation of 0.3 moles of NaI per mole of monomer reduces conductivity relative to that of polymer to which no salt has been purposely added.

500,352
PB85-229912 Not available NTIS

National Bureau of Standards, Gaithersburg, MD. Polymers Div.

Network Structure of Epoxies: 1. A Neutron Scattering Study.

Final rept.,
W. Wu, and B. J. Bauer. 1985, 5p
Pub. in Polymer Communication 26, p39-42 Feb 85.

Keywords: *Epoxy resins, *Molecular structure, *Neutron scattering, *Elastic scattering, Molecular weight, Deuterium compounds, Crosslinking, Thermosetting resins, Reprints, *Polymer chains, *Propanol/bis(epoxy propoxy)phenoxy).

The elastic neutron scattering technique was applied to elucidate the network structure of epoxies. A partially deuterated epoxy, the diglycidyl ether of Bisphenol A (DGEBA) was synthesized. It was then cured with di- and triamines based on polypropylene oxide chains for the neutron study. Prominent scattering peaks were observed in all the specimens over the q region within 1.2/Å. Furthermore, multiple scattering peaks were observed in the specimens cured with a diamine with rather high molecular weight.

500,353
PB85-229953 Not available NTIS

National Bureau of Standards, Gaithersburg, MD. Reactor Radiation Div.

Phonon Softening in a Mixed Layered System $\text{K}(\text{1-x})\text{Rb}(\text{x})\text{C}_8$.

Final rept.,
D. A. Neumann, H. Zabel, J. J. Rush, and N. Berk. 1984, 5p
Grant NSF-DMR83-04890
Sponsored by Conoco, Inc., Stamford, CT.
Pub. in Physical Review Letters 53, n1 p56-59, 2 July 84.

Keywords: *Inelastic scattering, *Neutron scattering, *Phonons, *Softening, *Graphite, Layers, Reprints, *Clathrate compounds.

By means of inelastic neutron scattering, the dispersion of the longitudinal (00q) phonon modes has been

Field 7—CHEMISTRY

Group 7D—Physical Chemistry

measured for the first time in the mixed layered compound $K(1-x)Rb(x)C8$ over the whole composition range $0 < x < 1$. From the optic and acoustic phonon branches interlayer force constants are derived which are strongly composition dependent. At $x = 0.65$ the elastic constant C_{33} shows an anomalous softening of more than 20%, which may be due to a composition-dependent charge transfer between the intercalant and graphite layers.

500,354

PB85-230019

Not available NTIS

National Bureau of Standards, Gaithersburg, MD. Polymers Div.

Phase Decomposition Phenomena of Polystyrene/Polyvinylmethylether.

Final rept.,

C. C. Han, M. Okada, Y. Muroga, B. J. Bauer, and Q. Tran-Cong. 1985, 6p

Pub. in Proceedings of the SPE Annual Technical Conference and Exhibition (43rd), ANTEC 85, Plastics 85, p306-310 1985.

Keywords: *Deuterium compounds, *Polystyrene, *Light scattering, *Decomposition reactions, Phase diagrams, Reaction kinetics, Nucleation, Experimental design, Plastics, Polyether resins, *Small angle scattering, *Poly(ether/methyl-vinyl), *Spinodal decomposition, Chemical reaction mechanisms.

Static and kinetic parameters of deuterated polystyrene/polyvinylmethylether blends before and during phase decomposition have been studied by the small angle neutron scattering and temperature jump light scattering techniques. Phase diagram, correlation length, critical exponent, binary interaction parameter together with spinodal temperatures and spinodal decomposition rate can all be studied in this approach. Two different decomposition mechanisms—spinodal and nucleation and growth—can be inferred from experimental results.

500,355

PB85-230407

Not available NTIS

National Bureau of Standards (NML), Gaithersburg, MD. Chemical Kinetics Div.

Ionic Hydrogen Bond and Ion Solvation. 2. Solvation of Onium Ions by One to Seven H₂O Molecules. Relations between Monomolecular, Specific, and Bulk Hydration.

Final rept.,

M. Mautner. 1984, 9p

See also Part 1, PB85-230415.

Pub. in Jnl. of the American Chemical Society 106, n5 p1265-1272 1984.

Keywords: *Enthalpy, *Water, *Hydration, Hydrogen bonds, Ions, Specific energy, pH, Chemical bonds, Reprints, *Onium ions, Proton affinity.

The relation between enthalpies of solvation of onium ions $BH(+1)$ by one water molecule, $-\Delta H(\text{sub } 0.1)$, and by four water molecules, $-\Delta H(\text{sub } 0.4)$, is constant for most onium ions: $\Delta H(\text{sub } 0.4)/\Delta H(\text{sub } 0.1)$ is 2.8 ± 0.1 for all oxonium ions and monoprotonic ammonium and pyridinium ions, and 3.1 ± 0.1 for polyprotonic ammonium ions. These relations, in conjunction with the correlation between $\Delta H(\text{sub } 0.1)$ and the proton affinity difference $\Delta PA = PA(B) - PA(H_2O)$, allow the prediction of the total four-molecule specific hydration energy $-\Delta H(\text{sub } 0.4)$ for all onium ions within the experimental accuracy of ± 3 kcal/mol. The observed (or predicted) four-fold specific relative hydration energies simulate closely the relative bulk hydration enthalpies for most ions. In other words, for most onium ions differential hydration effects are determined by the specific hydrogen-bonding interactions. Deviations are useful to identify bulk solvation effects. For example, such deviations indicate attenuated bulk solvation of ions with phenyl substituents.

500,356

PB85-230415

Not available NTIS

National Bureau of Standards (NML), Gaithersburg, MD. Chemical Kinetics Div.

Ionic Hydrogen Bond and Ion Solvation. 1. $NH(+1)-O$, $NH(+1)-N$, and $OH(+1)-O$ Bonds. Correlations with Proton Affinity. Deviations due to Structural Effects.

Final rept.,

M. Mautner. 1984, 9p

See also Part 2, PB85-230407.

Pub. in Jnl. of the American Chemical Society 106, n5 p1257-1264 1984.

Keywords: *Hydrogen bonds, *Molecular structure, *Solvation, Ions, Chemical bonds, Trends, Reprints, *Onium ions, *Proton affinity, Hydroxyl ions, Ammonium ions, Pyridium ions, Dimers.

In dimers $BH(+1) \cdots A$, a linear correlation is found between the bond dissociation energy $\Delta H(\text{sub } D)$ and the difference ΔPA between the proton affinities of the proton donor B and the proton acceptor A. The correlation applies for 48 $-NH(+1) \cdots O$ -dimers including a series with varying A and constant B, i.e., hydrates of ammonium and pyridium ions ($-NH(+1) \cdots OH_2$); a series with varying B and constant A, i.e., complexes $CH_3NH_3(+1) \cdots O$; and other dimers with ΔPA values varying from 9 to 70 kcal/mol and bond energies from 27 to 12 kcal/mol. The correlations are in accord with trends predicted by ab initio calculations of Desmeules and Allen. The correlations are reliable predictors of $BH(+1) \cdots A$ energies within experimental error limits. Deviations from the correlations help to identify special structural effects. Such effects include multiple hydrogen bonding, intramolecular hydrogen bonding, resonance, and steric crowding.

500,357

PB85-230423

Not available NTIS

National Bureau of Standards (NML), Gaithersburg, MD. Chemical Thermodynamics Div.

Ionic Hydrogen Bond. 1. Sterically Hindered Bonds. Solvation and Clustering of Protonated Amines and Pyridines.

Final rept.,

M. Mautner, and L. Sieck. 1983, 7p

See also Part 2, PB85-230431.

Pub. in Jnl. of the American Chemical Society 105, n10 p2956-2961 1983.

Keywords: *Hydrogen bonds, *Protonation, *Amines, *Pyridines, *Solvation, *Water, Stereochemistry, Hydration, Proton reactions, Entropy, Chemical bonds, Ions, Reprints, *Onium ions, *Proton affinity, Pyridium ions, Ammonium ions, Dimers.

The hydrogen-bonded dimer ions $BH(+1)-B$ and monohydrates $BH(+1)-H_2O$ of 2-alkylpyridines, 2,6-dialkylpyridines, and tertiary amines were investigated in the gas phase in the absence of solvent effects. The dissociation energies $\Delta H(\text{sub } D)$ of the dimers and hydrates are not affected by steric crowding. The authors observations may be summarized as follows: as long as there exists a single confirmation in which the hydrogen bond in $BH(+1)-B$ or $BH(+1)-H_2O$ can obtain optimal geometry, the bond strength is not weakened by steric crowding. However, steric crowding may result in major entropy effects due to the hindrance of internal rotors in the dimers and monohydrates.

500,358

PB85-230431

Not available NTIS

National Bureau of Standards (NML), Gaithersburg, MD. Chemical Thermodynamics Div.

Ionic Hydrogen Bond. 2. Intramolecular and Partial Bonds. Protonation of Polyethers, Crown Ethers, and Diketones.

Final rept.,

M. Mautner. 1983, 7p

See also Part 1, PB85-230423.

Pub. in Jnl. of the American Chemical Society 105, n15 p4906-4911 1983.

Keywords: *Hydrogen bonds, *Proton reactions, *Ethers, *Ketones, *Polyethers, *Intermolecular forces, Enthalpy, Stability, Thermochemistry, Entropy, Stereochemistry, Molecular rotation, Reprints, *Proton affinity.

Intramolecular hydrogen bonding in protonated di-, tri-, and tetraethers, as well as cyclic crown ethers, increases the proton affinities of these compounds vs. comparable monoethers. Thus, due to the stretched $OH(+1) \cdots O$ bond and small bond angle, here the 'hydrogen bond' may amount only to the electrostatic stabilization of the cis conformation, and rotation about the C-C bond is still allowed, although the barrier is increased by $-\Delta H(HB)$. The stability of the internal hydrogen bond decreases in the order diamines > diethers > diketones.

500,359

PB85-230654

Not available NTIS

National Bureau of Standards (NML), Gaithersburg, MD. Molecular Spectroscopy Div.

Product State and Kinetic Energy Distributions in the Ultraviolet Photodissociation of the NO-Ar van der Waals Molecule.

Final rept.,

D. S. King. Apr 85, 6p

Pub. in Jnl. of Chemical Physics 82, n8 p3629-3633, 15 Apr 85.

Keywords: *Ultraviolet spectroscopy, *Photodissociation, *Nitrogen oxide(NO), *Argon, *Reaction kinetics, Excitation, Doppler effect, Van der Waals equations, Fluorescence, Dissociation, Molecular rotational, Molecular vibration, Reprints, *Laser induced fluorescence.

The internal state and kinetic energy distributions of the X NO fragments formed from the ultraviolet photodissociation of the NO-Ar van der Waals species were obtained by laser-excited fluorescence techniques. The initially excited A NO-Ar rapidly dissociates to form X NO with little rotational excitation, with vibrational excitation determined by a Franck-Condon process, with a $\cos^2 \theta$ angular flux distribution (θ defined relative to the direction of polarization of the pump laser), and with a speed $v = 4.4 \times 10^5$ cm/s.

500,360

PB85-230662

Not available NTIS

National Bureau of Standards (NML), Gaithersburg, MD. Molecular Spectroscopy Div.

Energy Distribution in the Nitric Oxide Fragments from the ν_7 Vibrational Predissociation of NO-C₂H₄.

Final rept.,

D. S. King, and J. C. Stephenson. Jun 85, 4p

Pub. in Jnl. of Chemical Physics 82, n11 p5286-5288, 1 Jun 85.

Keywords: *Molecular vibration, *Nitrogen oxides(NO), *Molecular rotation, Energy transfer, Van der Waals equation, Fluorescence, Doppler effect, Reprints, *Laser excited fluorescence, *Laser spectroscopy.

The rotational level distribution of the NO fragments from the ν_7 vibrational dissociation of the NO-C₂H₄ van der Waals molecules was measured by laser excited fluorescence techniques to be Boltzmann in character, described by the rotational temperature 75 ± 15 K.

500,361

PB85-230670

Not available NTIS

National Bureau of Standards (NML), Gaithersburg, MD. Atomic and Plasma Radiation Div.

Analysis of the Fourth Spectrum of Tungsten (W IV).

Final rept.,

L. Iglesias, V. Kaufman, O. Garcia-Riquelme, and F. R. Rico. 1985, 12p

Pub. in Physica Scripta 31, p173-183 1985.

Keywords: *Tungsten, *Ionization, *Spectrographic analysis, *Ultraviolet spectroscopy, Molecular energy levels, Comparison, Least square methods, Reprints, Molecular configurations.

The spectrum of triply ionized tungsten (W IV) was produced in a sliding-spark discharge and recorded photographically on the NBS 10.7 m normal-incidence vacuum spectrograph in the 600-2600 Å spectral region. A total of 774 lines have been classified as transitions between these levels. Comparison of observed level values with those calculated in a least-squares fit shows an rms deviation of ± 50 cm for the even configurations and ± 250 cm for the odd ones.

500,362

PB85-230688

Not available NTIS

National Bureau of Standards (NML), Gaithersburg, MD. Molecular Spectroscopy Div.

Vibrational Deactivation of Surface OH Chemisorbed on SiO₂: Solvent Effects.

Final rept.,

E. J. Heilweil, M. P. Casassa, R. R. Cavanagh, and J. C. Stephenson. Jun 85, 17p

Pub. in Jnl. of Chemical Physics 82, n11 p5216-5231, 1 Jun 85.

Keywords: *Deactivation, *Molecular relaxation, *Surface chemistry, *Chemisorption, *Silicon dioxide, *Solvents, *Molecular vibration, Catalysis, Energy transfer, Lattice vibrations, Liquids, Infrared spectroscopy,

Spectrographic analysis, Line width, Reprints, *Hydroxyl radicals, Picosecond pulses.

Picosecond infrared transmission spectroscopy was used to directly measure the vibrational energy relaxation time T_1 of hydroxyl groups chemisorbed on the surface of colloidal silica (SiO₂). These observations are discussed in terms of the possible mechanisms of vibrational energy flow in these systems. The observed T_1 values demonstrate that the spectral linewidths (e.g., IR and Raman) observed for these surface vibrations are too large (by factors of 200-2000) to be caused solely by T_1 uncertainty broadening. The slow transfer of vibrational energy between surface and lattice vibrations may have important implications for surface chemistry.

500,363

PB85-230696

Not available NTIS

National Bureau of Standards (NML), Gaithersburg, MD. Molecular Spectroscopy Div.

Vibrational Energy Relaxation of Adsorbates on Surfaces.

Final rept.,

E. J. Heilweil, M. P. Casassa, R. R. Cavanagh, and J. C. Stephenson. 1985, 6p

Pub. in Proceedings of the Society of Photo-Optical Instrumentation Engineers 533, Ultrashort Pulse Spectroscopy and Applications, p15-19 1985.

Keywords: *Molecular vibration, *Surface chemistry, *Molecular relaxation, *Silicon dioxide, *Chemisorption, *Adsorbates, Spectroscopic analysis, Substrates, Infrared spectroscopy, Molecular energy levels, Reprints, *Lifetimes(Energy levels), Picosecond pulses, Hydroxyl radicals.

Picosecond infrared transient bleaching experiments have been performed to measure the population lifetime (T_1) of vibrationally excited ($v=1$) functional groups chemisorbed on high surface area colloidal silicas (SiO₂). The experimental method and results for vibrational modes of -OH, -OD, -NH₂ and -OCH₃ coordinated to surface silicon atoms and for the -BOH surface species are presented. Lifetimes for these groups at both vacuum and liquid interfaces indicate that the adsorbate degrees of freedom, chemical coordination and nearby substrate modes play an important role in damping vibrational energy. It is also surmised that the vibrational lifetime, especially that for the hydroxyl group ($T_1=150$ ps), is related to the chemical reactivity of adsorbates on surfaces.

500,364

PB85-230738

Not available NTIS

National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.

Pulsed Laser-Induced Thermal Desorption from Surfaces: Instrumentation and Procedures.

Final rept.,

D. R. Burgess, I. Hussla, P. C. Stair, R. Viswanathan, and E. Weitz. Nov 84, 7p

Contract N00014-79-C-0794

Pub. in Review of Scientific Instruments 55, n11 p1771-1776 Nov 84.

Keywords: *Laboratory equipment, *Surface chemistry, *Carbon monoxide, *Copper, Experimental design, Desorption, Reprints, *Time of flight mass spectroscopy, *Thermal desorption, *Laser induced desorption, Thermal pulse method, Procedures.

Instrumentation and procedures for performing pulsed laser-induced thermal desorption experiments are described. The influence of various instrumental parameters on the measured desorption signals is discussed. Proper conditioning of the desorption flux is shown to be a critical factor for obtaining desorption signals undistorted by the finite pumping speed of the apparatus. Instrumental effects are illustrated using data for pulsed laser desorption of CO from clean copper surfaces.

500,365

PB85-230753

Not available NTIS

National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.

Vibrational Energy Transfer Pathways in CH₃F Under Weak and Strong Excitation Conditions: A Comparison.

Final rept.,

V. A. Apkarian, J. M. Lindquist, and E. Weitz. Dec 84, 8p

Sponsored by National Science Foundation, Washington, DC.

Pub. in Chemical Physics Letters 112, n4 p328-334, 14 Dec 84.

Keywords: *Molecular vibrations, *Energy transfer, *Mathematical models, *Molecular energy levels, Excitation, Comparison, Fluorine organic compounds, Reprints, *Laser induced fluorescence, *Methane/fluoro.

Energy transfer processes in CH₃F have been reinvestigated under high excitation conditions with and without added rare gas via a mathematical model developed as a consequence of studies under low excitation. The model can be used to describe energy transfer under high excitation conditions with the inclusion of an additional state and energy transfer pathways coupling that state to others in the model. It is also concluded that multiple photon absorption takes place under high excitation conditions.

500,366

PB85-230779

Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

X-ray Interferometry: The Optical to Gamma-ray Connection.

Final rept.,

R. D. Deslattes. 1979, 18p

Pub. in Proceedings of the International Workshop on Neutron Interferometry, Grenoble, France, June 5-7, 1979, p399-415.

Keywords: *X rays, *Gamma rays, Quantum electrodynamics, Diffraction, *Interferometry.

In the recent past, it has been possible to complete an improved measurement chain connecting the hydrogen Rydberg with gamma-ray reference energies in the range $0.06 < E < 1.1$ MeV. Among other applications, these gamma-ray reference energies have been used to calibrate muonic X-ray spectra for tests of QED especially the vacuum polarization terms. Results of this improved calibration of the gamma-ray scale together with improved precision in the mesic X-ray to gamma-ray comparisons have resulted in the emergence of a pattern of substantial harmony between customary QED calculations and experiment. In a second application, the new gamma-ray values are used here as intermediate steps for the re-determination of several high Z X-ray lines where the X-ray to gamma-ray ratios have been previously established with high accuracies. In addition, a smaller number of X-ray lines have already been directly determined. Taken together these results produce an interim set of re-evaluated X-ray lines having higher accuracies than were previously available. When these are compared with recently available Hartree-Fock-Slater calculations, a systematic pattern of significant disagreement is evident.

500,367

PB85-230787

Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

Comparison of Relativistic Atomic SCF (Self-Consistent Field) Calculations with Improved Experimental Data.

Final rept.,

R. D. Deslattes, L. Jacobs, E. G. Kessler, and W. Schwitz. 1982, 10p

Pub. in Advances in X-ray Spectroscopy: A Reference Text in Honour of Professor Y. Cauchois, p144-152 1982.

Keywords: *X ray spectra, X ray spectroscopy, Gamma rays, Comparison.

The paper discusses the results of three comparisons between relativistic self-consistent field calculations and various experimental data. It is shown that by combining certain of the recently available optically referenced X-ray and gamma-ray wavelength measurements with a highly selected group of relative X-ray to X-ray and X-ray to gamma-ray comparisons, an improved, though quite limited, data base of transition energies can be obtained. The result shows deviations increasing with Z in a linear fashion. One possible origin for this result is discussed briefly.

500,368

PB85-230811

Not available NTIS

National Bureau of Standards (NML), Gaithersburg, MD. Gas and Particulate Science Div.

Radiocarbon: Nature's Tracer for Carbonaceous Pollutants.

Final rept.,

L. A. Currie, G. A. Klouda, and R. W. Gerlach. 1982, 22p

Pub. in Proceedings of the International Conference on Residential Solid Fuels, Environmental Impacts and Solutions, Portland, Oregon, June 1-4, 1981, p365-385 1982.

Keywords: *Radiocarbon dating, *Isotopic labeling, *Air pollution, *Environmental surveys, *Carbon isotopes, Carbon 12, Carbon 14, Urban areas, Rural areas, Biological aerosols, Residential buildings, Sampling, Sources, Combustion products, Wood, Biomass, Chemical analysis, Particle size, *Tracer studies, *Natural emissions, *Air pollution detection, Wood burning appliances.

Recent developments in radiocarbon dating techniques have made it feasible to determine ¹⁴C/¹²C ratios in samples containing milligram or even microgram quantities of carbon. As a result, it has become practicable to apply these techniques to the study of trace gases and particles in the atmosphere, as a means of resolving anthropogenic from natural source components. Interpretation of ¹⁴C data is straightforward: biospheric carbon (such as vegetation) is 'alive' with a ¹⁴C/¹²C ratio of about 1.5×10^{-10} to the 12th power, whereas fossil carbon is 'dead.' Beyond this dichotomous classification it becomes very interesting to combine the isotopic data with concurrent chemical data, as well as spatial and temporal distributions, in order to infer the strengths of specific sources of carbonaceous pollutants. A brief review will be presented of program on atmospheric gases and carbonaceous particles. For the latter, the authors have assayed individual chemical and size fractions, and samples collected in urban, rural, and remote locales. The biogenic carbon fraction -- presumably from wood-burning -- ranged from 10 percent to 100 percent for the urban samples analyzed.

500,369

PB85-235232

PC A03/MF A01

National Bureau of Standards (NML), Gaithersburg, MD. Office of Standard Reference Data.

Selected Tables of Atomic Spectra: A. Atomic Energy Levels - Second Edition. B. Multiplet Table - O III. Data Derived from the Analyses of Optical Spectra.

C. E. Moore. Jul 85, 35p

See also PB83-208942. Library of Congress catalog card no. 64-6074. Sponsored by Naval Research Lab., Washington, DC. E. O. Hulburt Center for Space Research.

Keywords: *Atomic spectra, *Atomic energy levels, *Oxygen, Tables(Data), *Multiplet energies.

The present publication is the eleventh section of a series being prepared in response to the read for a current revision of two sets of the author's tables containing data on atomic spectra is derived from analyses of optical spectra. As in the previous Sections, Part A, contains the atomic energy levels and Part B the multiplet tables. Section II includes these data for O III. The form of the presentation is described in detail in the text to Section I.

500,370

PB85-237329

PC A04/MF A01

National Bureau of Standards, Gaithersburg, MD.

Journal of Research of the National Bureau of Standards, Volume 90, Number 3, May-June 1985.

Jun 85, 64p

See also PB85-237337 through PB85-237360 and PB85-200129. Also available from Supt. of Docs as SN703-027-00004-1. Library of Congress catalog card no. 63-37059.

Keywords: *Research projects, Chemical analysis, Bioassay, Phase transformation, Laboratory equipment, Density(Mass/volume), Solids, Standards, Comparison, Volume, Design criteria, Performance evaluation, Fluids, Decomposition reactions, Sulfur hexafluoride, High temperature tests, High pressure tests, Reaction kinetics, Concentration(Composition), Electric corona, Electrophoresis, Chemical reaction mechanisms, Sulfur fluoride oxides, Sulfuryl fluoride, Thionyl fluoride, Thionyl tetrafluoride, PVT properties.

Contents:

Comparison of solid density standards between IMGC and NBS;

Field 7—CHEMISTRY

Group 7D—Physical Chemistry

Production rates for oxyfluorides SOF₂, SO₂F₂, and SOF₄ in SF₆ corona discharges;
A high temperature, high pressure reaction-screening apparatus;
Ways to standardization in electrophoresis are brought to light.

500,371
PB85-237337

(Order as PB85-237329, PC A04/MF A01)
Istituto di Metrologia Gustavo Colonnetti, Turin (Italy).
Comparison of Solid Density Standards between IMGC (Istituto di Metrologia 'Gustavo Colonnetti') and NBS (National Bureau of Standards),
A. Peuto, and R. S. Davis. 1 Mar 85, 11p
Prepared in cooperation with National Bureau of Standards, Gaithersburg, MD.
Included in Jnl. of Research of the National Bureau of Standards, v90 n3 p217-227 May-Jun 85.

Keywords: *Density(Mass/volume), *Solids, *Standards, Silicon, Comparison, Volume.

Solid-object density standards developed independently by the Istituto di Metrologia 'G. Colonnetti' (IMGC) and NBS, and traceable to SI units of length and mass, have been compared using a silicon transfer standard. Results agree to approximately .000001, which is consistent with the uncertainties assigned by the two laboratories.

500,372
PB85-237345

(Order as PB85-237329, PC A04/MF A01)
National Bureau of Standards, Gaithersburg, MD.
Production Rates for Oxyfluorides SOF₂, SO₂F₂, and SOF₄ in SF₆ Corona Discharges,
R. J. Van Brunt. 23 Jan 85, 25p
Included in Jnl. of Research of the National Bureau of Standards, v90 n3 p229-253 May-Jun 85.

Keywords: *Electric corona, *Reaction kinetics, *Sulfur hexafluoride, *Chemical analysis, Decomposition reactions, Chemical reactions, Trace elements, Gas chromatography, Mass spectroscopy, *Sulfur fluoride oxides, Chemical reaction mechanisms, Sulfuryl fluoride, Thionyl fluoride, Thionyl tetrafluoride.

The most abundant, long-lived stable gaseous species generated by corona discharges in SF₆ gas containing trace levels of O₂ and H₂O are the oxyfluorides SOF₂, SO₂F₂, and SOF₄. Absolute energy and charge rates-of-production of these and the minor products SO₂, OCS, and CO₂ have been measured at different total gas pressures from 100 kPa to 300 kPa and for discharges of different current, power, and polarity. The discharge current and time dependence of the production rates are discussed in terms of gas-phase mechanisms that have been proposed to explain previous observations of electrical, thermal, and laser-induced decomposition of SF₆ and SF₆/O₂ mixtures. Details of the chemical analysis procedures are given, and application of the results to the design of chemical diagnostics for SF₆-insulated, high-voltage apparatus is discussed.

500,373
PB85-237360

(Order as PB85-237329, PC A04/MF A01)
National Bureau of Standards, Gaithersburg, MD.
Ways to Standardization in Electrophoresis Are Brought to Light.
1985, 4p
Included in Jnl. of Research of the National Bureau of Standards, v90 n3 p259-262 May-Jun 85.

Keywords: *Electrophoresis, *Standards, *Meetings, Bioassay, Chemical analysis, Laboratory equipment.

A workshop entitled Electrophoresis Standardization: Approaches and Needs, drew 54 participants to the National Bureau of Standards (NBS) June 25, 1984. Co-sponsored by NBS and the Electrophoresis Society of the Americas, the meeting was hosted by the NBS Center for Analytical Chemistry. The first series of talks discussed various needs for standardization. Subsequent talks described how different laboratories approach standardization. Summaries of some of the talks are given in the review. A monograph containing edited versions of the papers was scheduled for release this spring.

500,374
PB86-101946

Not available NTIS
National Bureau of Standards (NML), Boulder, CO.
Quantum Physics Div.

Vibrational Excitation of D₂ by Low Energy Electrons.

Final rept.,
S. J. Buckman, and A. V. Phelps. Jun 85, 13p
Pub. in Jnl. of Chemical Physics 82, n11 p4999-5011, 1 Jun 85.

Keywords: *Molecular vibration, *Molecular energy levels, *Deuterium, Excitation, Cross sections, Hydrogen, Carbon dioxide, Carbon monoxide, Nitrogen, Reprints, *Electron molecule collision.

Excitation coefficients for the production of vibrationally excited D₂ by low energy electrons have been determined from measurements of the intensity of infrared emission from mixtures of D₂ and small concentrations of CO₂ or CO. The CO₂ and CO concentrations were chosen to allow efficient excitation transfer from the D₂ to the carbon containing molecule, but to minimize direct excitation of the CO₂ or CO. The measured infrared intensities were normalized to predicted values for N₂-CO₂ and N₂-CO mixtures at E/n where the efficiency of vibrational excitation is known to be very close to 100%. For our H₂-CO mixtures the excitation of CO via excitation transfer from H₂ is small compared to direct electron excitation of CO molecules. Published experiments and theories on electron-H₂ and electron-D₂ collisions are reviewed to obtain the cross sections used in the predictions.

500,375

PB86-102407
Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.
Observation of Autoionizing States of Beryllium by Resonance-Ionization Mass Spectrometry.
Final rept.,
C. W. Clark, J. D. Fassett, T. B. Lucatorto, L. J. Moore, and W. W. Smith. Jun 85, 6p
Contract DE-AC05-83ER60185
See also DE 85-009047.
Pub. in Jnl. of the Optical Society of America B 2, n6 p891-896 Jun 85.

Keywords: *Beryllium, Excitation, Atomic energy levels, Reprints, *Resonance ionization mass spectroscopy, *Autoionization, Rydberg series.

The authors have made the first reported observations of the Be 2p(sup 2) singlet S state, and of high-lying members of the Rydberg series 2pnd (sup 1)P(sup 0) (n < or = 16), by multiphoton resonance-ionization mass spectrometry (RIMS). The energy of the 1S state is compared with a number of theoretical predictions, which differ from one another over a range of about 0.75 eV. Good agreement is found when corrections are made for intershell electron correlations. These results show that precision spectroscopy can be performed by RIMS with samples of a few hundred atoms and that direct multiphoton excitation of autoionizing states may be a useful new addition to the existing catalog of resonance-ionization schemes.

500,376

PB86-102415
Not available NTIS
National Bureau of Standards (NML), Boulder, CO.
Quantum Physics Div.
Ion Chemistry in Silane dc Discharges.
Final rept.,
H. Chatham, and A. Gallagher. 1 Jul 85, 11p
Sponsored by Solar Energy Research Inst., Golden, CO.
Pub. in Jnl. of Applied Physics 58, n1 p159-169, 1 Jul 85.

Keywords: *Silane, *Ionization, *Chemical reactions, *Electric discharges, Comparison, Mass spectroscopy, Reprints, *Ion molecule interactions.

The ion production and reactions in dc silane discharges are calculated. It is noted that almost all ion production and reaction occur in the cathode sheath region for typical low-pressure silicon-deposition discharges, so that the calculation considers ion production, drift, and reactions in the sheath region. Sheath models, for inert gas discharges, that utilize local and nonlocal electron energy distributions are compared, and one is adapted to silane conditions. The distribution of ion species (Si(sub l)H(sub m)(+1)) arriving at the cathode is calculated for a range of discharge pressures and currents, for comparison to mass spectrometer measurements. However, the authors do not make quantitative comparisons to reported observations due to sampling-bias issues that have not been taken into account.

500,377

PB86-102423
Not available NTIS
National Bureau of Standards (NML), Boulder, CO.
Quantum Physics Div.
Nonadiabatic Molecular Collisions. 2. A Further Trajectory-Surface-Hopping Study of the ArH₂(+1) System.
Final rept.,
S. Chapman. May 85, 11p
Pub. in Jnl. of Chemical Physics 82, n9 p4033-4043, 1 May 85.

Keywords: *Surface chemistry, Mathematical models, Diatomic molecule, Experimental design, Comparison, Reprints, Ion molecule interactions, *Molecule molecule collisions, *Ion molecule collisions.

Both charge transfer and chemical reaction are studied for the reactants Ar(+1) + H₂, Ar + H₂(+1), and Ar + D₂(+1), using the trajectory-surface-hopping model with diatomics-in-molecules 2A surfaces for ArH₂(+1). Results are compared with a number of recent experiments. Agreement with experiment is generally satisfactory. The reactions are direct. The Ar(+1) + H₂ yields ArH(+1) + H reaction is well characterized as a stripping process. Charge transfer occurs predominantly by long-range electron jump. Points of disagreement with experiment are discussed in the light of the approximations in the surface and the TSH model.

500,378

PB86-102456
Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.
Remarks on the Translational Diffusion Coefficient of Relatively Short Chains.
Final rept.,
A. Z. Akcasu, and C. M. Guttman. 1985, 6p
Pub. in Macromolecules 18, n5 p938-943 1985.

Keywords: *Molecular structure, *Mathematical models, Diffusion coefficients, Hydrodynamic configurations, Reprints, *Polymer chains.

The expansion of the hydrodynamic radius R(sub H) in inverse powers of N(sup 1/2) is presented for three chain models which allow only for local structure along the chain. The effect of chain stiffness is included in one of the models. Formulas are presented to interpret R(sub H) data for relatively short chains. The approach to the Gaussian chain limit as N approaches infinity is discussed.

500,379

PB86-102944
Not available NTIS
National Bureau of Standards (NML), Boulder, CO.
Quantum Physics Div.
Rapid Collisional Quenching of the N=1, nu=2 level of the H₂(cu c)pi(sub u) Metastable State by H₂.
Final rept.,
H. Tischer, and A. V. Phelps. Jul 85, 5p
Pub. in Chemical Physics Letters 117, n6 p550-554 Jul 85.

Keywords: *Hydrogen, *Reaction kinetics, *Metastable state, Electric discharges, Quenching distance, Reprints, *Molecule molecule collisions, *Laser spectroscopy.

The rate coefficient for collisional quenching of the N = 1, nu = 2 level of the H₂(cu c pi(sub u)) metastable state by H₂ is measured to be (2.0 +/- or - 0.2) x 10 to the -15th power cu m/s at 300 K. The metastables are produced by an electric discharge, radiatively quenched by a pulsed laser and the recovery of metastable population monitored by cw dye laser absorption.

500,380

PB86-102969
Not available NTIS
National Bureau of Standards (NML), Boulder, CO.
Quantum Physics Div.
Laser-Assisted Charge-Transfer Reactions (Li(+3) + H): Coupled Dressed-Quasimolecular-State Approach.
Final rept.,
T. S. Ho, C. Laughlin, and S. I. Chu. Jul 85, 11p
Pub. in Physical Review A 32, n1 p122-132 Jul 85.

Keywords: *Hydrogen, Perturbation theory, Hamiltonian functions, Reprints, *Lithium ions, *Dressed quasi-

molecular states, *Laser enhanced ionization, Generalized Van Vleck theory, Floquet theory.

A semiclassical coupled dressed-quasimolecular-states (DQMS) approach is presented for nonperturbative treatment of multichannel charge-transfer reactions at low collision velocities and high laser intensities, incorporating the implementation of the generalized Van Vleck (GVV) nearly degenerate perturbation theory. The GVV technique allows block partitioning of the infinite-dimensional Floquet Hamiltonian into a finite-dimensional model DQMS space, and thereby reduces greatly the number of effective coupled channels. Further, the GVV-Floquet basis allows minimization of the (usually large in amplitude) field-induced nonadiabatic radial couplings without the need to explicitly construct the transformation between the adiabatic and diabatic DQMS basis. This yields a new set of coupled GVV-DQMS equations (neither adiabatic nor diabatic) which are particularly convenient for multichannel calculations.

500,381
PB86-102977 Not available NTIS
National Bureau of Standards (NML), Boulder, CO.
Quantum Physics Div.
Ab Initio Calculations of Low-Energy Electron Scattering by HCN Molecules.
Final rept.,
A. Jain, and D. W. Norcross. Jul 85, 10p
Sponsored by Department of Energy, Washington, DC.
Pub. in Physical Review A32, n1 p134-143 Jul 85.

Keywords: *Cyanides, *Molecular rotation, *Electron scattering, Mathematical models, Comparison, Experimental design, Excitation, Hartree Fock approximation, Reprints, *Electron molecule collisions.

The authors report results for vibrationally elastic scattering over the energy range 0.0006-11.6eV. The interaction potential is composed of a near-Hartree-Fock static term plus a parameter-free model of the correlation-polarization potential. The exchange interaction is included exactly through a separable expansion. Results with a model-exchange potential (free-electron-gas plus orthogonalization) are also reported. A resonance appears in pi symmetry near 2.7eV (width 1.9eV) that may be the same feature observed in several experiments. In the model-exchange calculation the pi resonance is shifted toward higher energy (3.8eV, width 2.4eV). The sigma symmetry was also found to be very sensitive to the treatment of exchange and to the effect of polarization. Differential and rotational excitation cross sections are evaluated in the multipole-extracted adiabatic-nuclei approximation. Results are compared with the available experimental and theoretical data.

500,382
PB86-103025 Not available NTIS
National Bureau of Standards (NML), Boulder, CO.
Time and Frequency Div.
Hyperfine Structure of the 2p doublet P(sub 1/2). State in (sup 9)Be(+1).
Final rept.,
J. J. Bollinger, J. S. Wells, D. J. Wineland, and W. M. Itano. 1985, 4p
Sponsored by Air Force Office of Scientific Research, Bolling AFB, DC., and Office of Naval Research, Arlington, VA.
Pub. in Physical Review A 31, n4 p2711-2714 Apr 85.
Keywords: *Hyperfine structure, *Atomic energy levels, Excitations, Magnetic dipoles, Reprints, *Beryllium ions.

An optical-optical double resonance technique has been used on beryllium ions stored in a Penning trap to measure the magnetic dipole hyperfine interaction constant A(sub 1/2) of the 2p double P(sub 1/2) level in (sup 9)Be(+). The measured value of A(sub 1/2) = -118.6(3.6) MHz is in good agreement with theoretical calculations.

500,383
PB86-103470 PC A05/MF A01
National Bureau of Standards, Gaithersburg, MD.
NBS (National Bureau of Standards): Materials Measurements. Annual Report for 1 April 1984-31 March 1985.
J. R. Manning. Jul 85, 98p NBSIR-85/3217
Contract NASA-H-27954-B
See also PB80-223159.

Keywords: *Interfacial tension, *Convection, *Thermodynamic properties, Gallium, Silicon, Impurities, Re-

duced gravity, *Directional solidification, Temperature dependence, Levitation.

The report describes NBS work for NASA in support of NASA's Microgravity Science and Applications Program under NASA Government Order H-27954B (Properties of Electronic Materials) covering the period April 1, 1984 to March 31, 1985. The work has been carried out in three independent tasks: Task 1--Surface Tensions and Their Variations with Temperature and Impurities; Task 2--Convection during Unidirectional Solidification; Task 3--Measurement of High Temperature Thermodynamic Properties. The results for each task are given separately in the body of the report.

500,384
PB86-103496 PC A04/MF A01
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Building Technology.
Molecular and Microstructural Factors Affecting Mechanical Properties of Polymeric Cover Plate Materials.
E. J. Clark. Jul 85, 67p NBSIR-85/3197
Sponsored by Department of Energy, Washington, DC.
Office of Solar Heat Technologies.

Keywords: *Mechanical properties, *Polymers, *Microstructure, *Degradation, *Coverings, Reviews, Deformation, Structural analysis, Plastics, Molecular structure, Molecular weight, Crosslinking, Materials tests.

The paper reviews the dependence of mechanical properties of polymers on various microstructural factors. The microstructural and molecular factors considered are: molecular weight, crystallinity, crosslinking, branching, copolymerization, plasticization, orientation, and residual stresses. The types of mechanical properties considered are: direct loading, fatigue, creep, wear and abrasion, and environmental stress cracking. The effects of polymer deformation and fraction at the molecular level are discussed. Cracking, crazing, and shear yielding are described. Polymeric cover plate materials are discussed and their degradation reviewed. Methods to measure microlevel changes in polymers are identified.

500,385
PB86-103603 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.
Electron Spectrometry Study of Associative and Penning Ionization in Laser Excited Sodium Vapor.
Final rept.,
B. Carre, G. Spiess, J. M. Bizau, P. Dhez, and P. Gerard. 1 Nov 84, 6p
Pub. in Optics Communications 52, n1 p29-34, 1 Nov 84.

Keywords: *Ionization, *Electronic spectra, *Atomic energy levels, Excitation, Synchrotron radiation, Reprints, *Sodium atoms, *Penning effect, *Laser enhanced ionization.

The first observation, by electron spectrometry, is reported in laser-excited sodium vapor of the primary low energy electrons produced by associative ionization and by Penning ionization of sodium atoms in highly excited nl states. The sequential heating of these primary electrons has been observed in 1, 2, or 3 superelastic collisions with Na (3p) atoms. The variation of associative ionization was measured as a function of the excited state density by using inner-shell photoionization produced by synchrotron radiation.

500,386
PB86-103629 Not available NTIS
National Bureau of Standards (NML), Boulder, CO.
Quantum Physics Div.
Electron Impact Excitation of Ions in the Magnesium Sequence: Fe XV.
Final rept.,
R. B. Christensen, D. W. Norcross, and A. K. Pradhan. Jul 85, 12p
Sponsored by Department of Energy, Washington, DC.
Pub. in Physical Review A32, n1 p93-104 Jul 85.

Keywords: *Quantum theory, Excitation, Hamiltonian functions, Reprints, *Electron ion interactions, *Electron ion collisions, *Magnesium ions.

Intermediate-coupling collision strengths are calculated for all transitions between the states. Calculations are carried out in a ten-state distorted-wave approximation. Resonance effects are considered by using

multichannel quantum-defect theory, and relativistic effects in the target Hamiltonian are taken into account in the Breit-Pauli formulation. Term coupling among the target states also affects several transitions considerably. Present results are compared with previous calculations; some significant differences are noted. The new results suggest a serious discrepancy between calculated and observed relative intensities of the 284.2-A (resonance) and 417.3-A (intercombination) lines for Fe XV in the Sun, but will reduce the discrepancy for this ratio for other Mg-like ions observed in tokamak plasmas.

500,387
PB86-105848 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD.
Determination of Trace Element Forms in Solvent Refined Coal Products.
Final rept.,
B. S. Carpenter, and R. H. Filby. 1982, 14p
Pub. in Proceedings of the American Nuclear Society Conference, At. Nuclear Methods Fossil Energy Research, p83-96 1982.

Keywords: *Trace elements, *Chemical analysis, Coal liquefaction, Metals, Neutron activation analysis, Chromatographic analysis, Atomic spectroscopy, Metal containing organic compounds, Complex compounds, *SRC process, *SRC II process, *Air pollution detection, High performance liquid chromatography, Heavy metals, Gel permeation chromatography.

The Solvent Refined Coal Processes SRC I and SRC II are designed to produce low ash, low sulfur solid (SRC I) and liquid fuels (SRC II) from coal. Both processes are currently undergoing scale-up to a 6000 tons per day demonstration plant stage. The fate and distribution of Ti, V, Ca, Mg, Al, Cl, Mn, As, Se, Sb, Hg, Br, Ni, Co, Cr, Fe, Na, Rb, Cs, K, Sc, Eu, Sm, Ce, La, Sr, Ba, Th, Hf, Ta, Zr and Cu in the SRC I and SRC II processes have been determined using neutron activation analysis. The nature of the chemical species of several elements has been investigated using fission track analysis for U and a combination of gel permeation chromatography, HPLC, activation analysis and atomic absorption spectroscopy for other elements. These elements were probably present as metal-organic complexes or complexed in the asphaltene or preasphaltene structure. The nature of these complexes could not be established, but for Ti and V there is a strong possibility of phenolic-type complexes.

500,388
PB86-109949 PC A03/MF A01
National Bureau of Standards, Boulder, CO.
Glass Fiberblanket SRM (Standard Reference Material) for Thermal Resistance.
Final rept.,
J. G. Hust. Sep 85, 30p NBS/SP-260/103
Also available from Supt. of Docs as SN003-003-02687-5. Library of Congress catalog card no. 85-600582.

Keywords: *Glass fibers, *Thermal resistance, *Thermal insulation, *Standards, Thermal conductivity, *Blankets(Bedding), *Standard reference materials.

The apparent thermal conductivity data that provide the basis for the certification of glass fiberblanket as an SRM of thermal resistance are reported and analyzed. Detailed analysis and intercomparisons of NBS and other published data are given. These data are represented by an equation describing the dependencies of the data on temperature and density. Certified values of thermal resistance are given for temperatures from 100 to 330 K and densities from 10 to 16 kg/cu m.

500,389
PB86-109956 PC A04/MF A01
National Bureau of Standards (NML), Gaithersburg, MD.
Chlorine Content of Municipal Solid Waste from Baltimore County, MD, and Brooklyn, NY.
K. L. Churney, A. E. Ledford, S. S. Bruce, and E. S. Domalski. Sep 85, 66p NBSIR-85/3213
Contract DE-A101-83-CE30801
Sponsored by Department of Energy, Washington, DC., and New York City Dept. of Sanitation.

Keywords: *Chlorine, *Chemical analysis, *Sulfur, *Materials tests, Sampling, Sites, Concentration(Composition), Air pollution, Paper prod-

Field 7—CHEMISTRY

Group 7D—Physical Chemistry

ucts, Composite materials, *Municipal wastes, Air pollution sampling, Air pollution detection, Solid wastes, Baltimore County(Maryland), Brooklyn(New York), Refuse derived fuels.

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 component which contributed the largest fraction to the chlorine content in Baltimore County, MD was the paper fraction while in Brooklyn, NY, the plastics fraction provided the major contribution (0.46 mass % or 52% of the total chlorine). Chemical analyses for sulfur content were performed on composite samples for each day of sampling at the two sites. American Society for Testing and Materials (ASTM) standard methods for sulfur, total chlorine, and water soluble chlorine contents, developed for refuse-derived fuel, were used in performing the analyses.

500,390

PB86-110129 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Center for Fire Research.
Investigation of Wood Pyrolysis Using Solid State ¹³C Nuclear Magnetic Resonance.

Final rept.,
W. L. Earl. 1982, 17p
Pub. in Proceedings of 1981 International Conference on Residential Solid Fuels, Environmental Impacts and Solutions, Portland, OR., June 1-4, 1981, p772-778 1982.

Keywords: *Nuclear magnetic resonance, *Wood, *Combustion, *Char, Pyrolysis, Carbon 13, Isotopic labeling, Chemical analysis, Heat transfer, Aromatic polycyclic hydrocarbons, *Air pollution detection.

The present state of the art in ¹³C NMR of solids yields spectra with narrow lines which are useful for obtaining chemical information in intractable solids. These NMR techniques have been applied to the analysis of a series of chars obtained by subjecting spruce and oak wood to temperatures between 550 and 660 K in nitrogen. The NMR spectra obtained indicate that the cellulose starts to decompose before lignin but by 615 K both components are decomposing. The solid char formed is highly aromatic, probably being composed of a large variety of poly-nuclear aromatics. It is suggested that the rate of pyrolysis is determined by the rate of heat transfer in woody samples.

500,391

PB86-110145 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Gas and Particulate Science Div.
Empirical Quantitation In Raman Microprobe Analyses.

Final rept.,
E. S. Etz. 1981, 6p
Pub. in Proceedings of Annual Conference on Microbeam Analysis Society (16th), Vail, CO., July 13-17, 1981, p73-78.

Keywords: *Raman spectroscopy, *Microanalysis, *Probes, Chemical analysis, Calcium phosphates, Bioassay, Elastic scattering, Forecasting, Sampling.

A non-rigorous exposition of the problems of quantitation in Raman microprobe analysis is presented. The micro-Raman scattering characteristics are reviewed, highlighting analytical advantages and limitations as they apply to the considerations for quantitative analysis. The concepts of quantitation valid for bulk samples are extended to scattering from microscopic samples and the difficulties noted. The conclusions that can be drawn from the results of current on elastic scattering theories are formulated and taken as a basis for the argument that empirical approaches are likely to produce adequate quantitative data for present requirements. The case for calibration methods based on the use of standards is presented by a discussion of NBS results obtained in the quantitative estimation of carbonate contents on biological apatites. Future directions are noted that promise to advance the prospects for micro-Raman quantitation.

500,392

PB86-110178 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Chemical Stability and Corrosion Div.

Thermodynamic Models of Alkali-Metal Vapor Transport In Silicate Systems.

Final rept.,
J. W. Hastie, W. S. Horton, E. R. Plante, and D. W. Bonnell. 1982, 11p
Pub. in High Temperature - High Pressures 14, n6 p669-679 1982.

Keywords: *Thermodynamics, *Mathematical models, *Transport properties, *Alkaline earth metals, *Silicates, *Liquid theory, Experimental design, Vaporizing, High temperature tests, Solutions,

A thermodynamic data base has been developed for liquid/solid mixtures containing K₂O, Al₂O₃ and SiO₂. Together with the hypothesis of Ideal Mixing of Complex Phases (IMCP) this data base reproduces experimental activity data, expressed here for convenience in terms of P(sub K), over a wide range of composition and temperature. The authors are confident that the model (IMCP + data base) can be applied to the prediction of solution thermodynamics, vaporization rates, and perhaps even phase stability diagrams for systems not readily amenable to experimental study. As a future extension of this work, they will progressively extend the data base and provide model validation tests for systems containing Na₂O, CaO, MgO and Fe₂O₃, in addition to the components considered here.

500,393

PB86-110830 PC A07/MF A01
National Bureau of Standards (NML), Gaithersburg, MD. Center for Analytical Chemistry.
Summary of the Coal, Ore, Mineral, Rock, and Refractory Standards Issued by the National Bureau of Standards.

T. E. Gills, and R. Mavrodineanu. Sep 85, 137p
NBS/SP-260/97
Also available from Supt. of Docs as SN003-003-02688-3. Library of Congress catalog card no. 85-600577.

Keywords: *Coal, *Nonmetalliferous minerals, *Minerals, *Rocks, *Refractories, *Chemical analysis, *Metalliferous minerals, Standards, Beneficiation, *Standard reference materials, Listings.

The publication is a summary of the coal, ore, mineral, rock, and refractory standards issued by NBS as Standard Reference Material (SRM's). The material, composition, certification, use, and remarks concerning each of the SRM's described are presented in tabular form. Copies of the certificates of these SRM's are contained in the appendix for more detailed information.

500,394

PB86-110855 PC A09/MF A01
National Bureau of Standards (NML), Boulder, CO. Time and Frequency Div.
Trapped Ions and Laser Cooling: Selected Publications of the Ion Storage Group of the Time and Frequency Division, NBS, Boulder, CO.

Technical note,
D. J. Wineland, W. M. Itano, J. C. Bergquist, and J. J. Bollinger. Jul 85, 195p NBS/TN-1086
Also available from Supt. of Docs as SN003-003-02666-2. Sponsored by Office of Naval Research, Arlington, VA., and Air Force Office of Scientific Research, Bolling AFB, DC.

Keywords: *Frequency standards, *Atomic spectroscopy, Time standards, Atomic clocks, *Ion traps, *Laser cooling, Laser spectroscopy, Penning traps.

The report contains selected publications of the Ion Storage Group of the Time and Frequency Division, NBS, Boulder, Colorado. Partial contents include: Laser Cooling of Atoms; Spectroscopy of a Single Mg(+) Ion; Laser Cooling of Ions Stored in Harmonic and Penning Traps; Spectroscopy of Stored Ions; Frequency Standard Research Using Stored Ions; Laser-Cooled-Atomic Frequency Standard.

500,395

PB86-110897 PC A06/MF A01
National Bureau of Standards (NML), Gaithersburg, MD. Center for Analytical Chemistry.
Handbook for SRM (Standard Reference Materials) Users.

Final rept.,
J. K. Taylor. Sep 85, 101p NBS/SP-260/100
Also available from Supt. of Docs as SN003-003-02689-1. Library of Congress catalog card no. 85-600576.

Keywords: *Handbooks, *Chemical analysis, *Guidelines, Performance evaluation, Quality assurance, Measurements, Calibrating, Statistical analysis, Laboratory equipment, *Standard reference materials.

The handbook was prepared to provide guidance for the use of Standard Reference Materials (SRM's) to provide an accuracy base for chemical measurements. The general concepts of precision and accuracy are discussed and their realization by quality assurance of the measurement process. General characteristics of SRM's are described and guidance is given for their selection for specific applications. Ways to effectively use SRM's are recommended, utilizing control charts to evaluate and monitor measurement accuracy. Appendices provide statistical guidance on the evaluation of measurement uncertainty.

500,396

PB86-111358 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Gas and Particulate Science Div.
Quantitative Electron Probe Microanalysis of Fly Ash Particles.

Final rept.,
R. L. Myklebust, J. A. Small, and D. E. Newbury. 1982, 10p
Pub. in Proceedings of the American Nuclear Society Conference on Atomic and Nuclear Methods in Fossil Energy Research, Mayaguez, PR., December 1-4, 1980, p285-294 1982.

Keywords: *Fly ash, *Particles, *Chemical analysis, *Electron probes, X-ray analysis, Air pollution, *Air pollution detection, Standard reference materials.

Fly ash particles or other similar particles may be quantitatively analyzed with a flat sample matrix correction method that has been modified to include the peak-to-background ratio for each element as a normalizing factor. The effects of the different matrix corrections on particles is discussed. Examples of analyses of standard reference material glass particles by both a standard matrix correction program (FRAME C) and a modified correction program (FRAME P) are presented as well as analyses of fly ash (SRM-1633).

500,397

PB86-111366 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Beam Broadening in the Analytical Electron Microscope.

Final rept.,
D. E. Newbury. 1982, 5p
Sponsored by Microbeam Analysis Society, Bethesda, MD.
Pub. in Proceedings of Annual Conference of Microbeam Analysis Society (17th), Washington, DC., August 9-13, 1982, p79-83.

Keywords: *Electron microscopes, *X ray analysis, Scattering cross sections, Elastic scattering, Mathematical models, Gold, *Beam foil spectroscopy.

Beam spreading in thin foils occurs in the analytical electron microscope as a result of elastic scattering. Various models which attempt to quantify the dimensions of the spreading are cataloged: analytic single, plural, and multiple scattering models, thermal diffusion analog model, and Monte Carlo electron trajectory simulations. Despite apparent differences in the assumptions of the models, calculated results show only a 30% range for a gold foil. This similarity is ascribed to a basic dependence on the single scattering cross section for all of the models.

500,398

PB86-111382 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Gas and Particulate Science Div.
Monte Carlo Electron Trajectory Calculations of X-ray Generation In Tilted, Solid Specimens.

Final rept.,
D. E. Newbury, and R. L. Myklebust. 1981, 3p
Pub. in Proceedings of Annual Conference on Microbeam Analysis Society (16th), Vail, CO., July 13-17, 1981, p175-177.

Keywords: *Solids, *X-ray analysis, *Monte Carlo method, Electron probes, Backscattering, Sampling, Numerical solution.

Monte Carlo electron trajectory calculations provide a useful technique to obtain information on electron beam interactions in solids in situations in which direct

experimental measurements are difficult or impossible. In the present work, electron interactions have been simulated in solid specimens tilted at various angles to the incident beam. Parameters which describe certain aspects of x-ray generation, including the characteristic-bremsstrahlung ratio (peak-to-background), loss of generation due to electron backscattering, and the x-ray absorption effect, have been determined in support of the development of methods for quantitative x-ray micro-analysis of tilted samples.

500,399
PB86-111713 Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Chemical Engineering Science Div.
Measurements of the Viscosities of Saturated and Compressed Liquid Normal Butane and Isobutane. Final rept., D. E. Diller, and L. J. Van Poolen. Jan 85, 20p
Sponsored by Gas Research Inst., Chicago, IL., and Department of Energy, Washington, DC.
Pub. in Int. J. Thermophysics 6, n1 p43-62 Jan 85.

Keywords: *Viscosity, Compressed liquid, Density(Mass/volume), Saturation, Piezoelectric crystals, Butanes, Reprints, *Butane, *Propane/methyl, Numerical solution.

The shear viscosity coefficients of saturated and compressed liquid normal butane and isobutane have been measured with the torsional piezoelectric crystal method at temperatures between 115 and 300 K and at pressures to 30 MPa. The measurements have been correlated with a modified Hildebrand equation. The experimental error is estimated to be smaller than 3%. The measurements of normal butane and isobutane have been compared with a global extended corresponding states model and with each other. Differences between measured and calculated viscosities are discussed.

500,400
PB86-111747 Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
Excited States Created in Charge Transfer Collisions between Atoms and Highly Charged Ions. Final rept., R. K. Janev. 1983, 14p
Pub. in Proceedings of International Symposium on Production and Physics of Highly Charged Ions, Stockholm, Sweden, June 1-5, 1982, Physica Scripta T3, p208-221 1983.

Keywords: *Atomic energy levels, Excitation, Electron transfer, Electron capture, *Atom ion collisions, *Charge exchange reactions.

A survey of theoretical achievements and problems in the study of formation of excited states in atom-highly charged ion charge-exchange collisions is presented. Both one- and many-electron colliding systems are considered. Apart from the basic single electron transfer reactions, other multi-electron transition processes leading to creation of excited product states are also discussed. The theoretical data on the final state distributions of capture electrons are critically analyzed and the problems which require further investigations are emphasized.

500,401
PB86-111754 Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
Electron Capture into Excited States in H + Ar(+18), Kr(+36) and Xe(+54) Charge Transfer Collisions. Final rept., R. K. Janev, and D. S. Belic. 1983, 3p
Pub. in Proceedings of International Symposium on Production and Physics of Highly Charged Ions, Stockholm, Sweden, June 1-5, 1982, Physica Scripta T3, p246-248 1983.

Keywords: *Electron capture, *Atomic energy levels, Excitations, Electron transfer, Mathematical models, *Charge exchange reactions, *Atom ion collisions.

Partial cross sections for electron capture into specific final state principal shells in H + Ar(+18), Kr(+36) and Xe(+54) collisions are calculated. A multi-channel Landau-Zener model, which includes also the rotational transitions in the ionic channels, is employed. The calculations are performed in the energy range from .01 to 100 keV/amu.

500,402
PB86-111762 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Gas and Particulate Science Div.
Round Robin Test on ELS (Electron Energy Loss Spectroscopy) Quantitation. Final rept., D. C. Joy, and D. E. Newbury. 1981, 3p
Pub. in Proceedings of Annual Conference of the Microbeam Analysis Society (16th), Vail, CO., July 13-17, 1981, p178-180 1981.

Keywords: *Carbon, *Chemical analysis, Electron microscopy, *Electron energy loss spectroscopy, *Scanning electron microscopy, *Transmission electron microscopy.

A round robin test has been performed for analysis by electron energy loss spectroscopy on the analytical electron microscopy. Carbon thin films were measured and several parameters were calculated from the spectrum, including the number of atoms per square centimeter of target, the pre-absorption and post-absorption edge, exponential background parameters, and the total spectrum intensity to zero-loss intensity ratio. Good agreement for these parameters among three of the participating laboratories was noted. Substantial disagreement in two other measurements is attributed to errors in data collection and/or reduction.

500,403
PB86-111796 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Molecular Spectroscopy Div.
Pump-Probe Techniques Applied to Spectroscopic and Kinetic Studies of Radicals. Final rept., D. S. King, and R. F. Wormsbecher. 1981, 6p
Sponsored by SPIE-The International Society for Optical Engineering, Bellingham, WA.
Pub. in Proceedings of the SPIE Laser Spectroscopy for Sensitive Detection Conference, Washington, DC., April 23-24, 1981, v286 p111-116.

Keywords: *Free radicals, *Reaction kinetics, *Electron probes, Dissociation, Molecular relaxation, Mass transfer, Electronic pumping, Combustion products, Gas analysis, *Laser spectroscopy, Air pollution detection, Nitride/methyl, Atmospheric chemistry.

In response to recent interests in laser applications to monitoring the role of radical species in combustion and atmospheric chemistry several new techniques have been developed. In this paper the authors discuss a laser-probe technique utilized in our lab to obtain spectroscopic data for such in situ or long range studies and kinetic data on mass transport, vibrational and rotational relaxation, and chemical delay. The work utilizes a pulsed photolysis (excimer, YAG, CO₂) laser to generate the radical in a well defined spatial region and a second probe (tunable dye) laser delayed in time. Applications of this technique to relaxation processes in CF₂ and to new spectroscopic data on OCH₃ will be discussed.

500,404
PB86-111804 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Estimating the Impact of Atmospheric Carbonaceous Particulates on Urban and Rural Environments by Radiocarbon Measurements. Final rept., G. Klouda, L. Currie, R. Gerlach, R. Continetti, and G. Tompkins. 1982, 18p
Pub. in Proceedings of Residential Wood and Coal Combustion Specialty Conference, Louisville, KY., March 1-2, 1982, Spec. Conf. Proc. SP-45, p189-206.

Keywords: *Environmental surveys, *Radioactive age determination, *Radiocarbon dating, Isotopic labeling, Mass spectroscopy, Chemical analysis, Assessments, Particles, Urban areas, Rural areas, *Accelerator mass spectroscopy, *Air pollution detection, Natural emissions, Wood burning appliances, Tracer studies.

Natural radiocarbon ((14)C) has been extensively utilized to decipher the history of the earth and more recently to reconstruct episodes of environmental pollution. Radiocarbon measurements of atmospheric carbonaceous particulates via low-level counting (llc) have demonstrated its usefulness as a unique discriminator of fossil and biogenic contributions to the degradation of air quality. In addition, the revolution in ((14)C) single atom counting by Accelerator Mass Spectrometry (AMS) will allow one to investigate indi-

vidual organic compounds for source identification. Preliminary steps in development of an analytical technique for AMS sample preparation are discussed. The dichotomous model of fossil/biogenic source contributions to air pollution is resolvable by identifying the fraction of contemporary carbon of carbonaceous particulates through radiocarbon measurements. Studies currently underway include characterizing the rural forested areas of Abastumani, USSR and the Shenandoah Valley, Virginia and source assessment of particles collected at Pt. Barrow, Alaska for examining the 'Arctic Haze' episodes. The power of ((14)C) as an environmental tracer is being enhanced by including this information in the Receptor Model approach. Research is underway to produce a simulated data set for fictitious receptor sites which can be used to validate existing models.

500,405
PB86-111820 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Inorganic Materials Div.
Applications of Equilibrium Diagrams to Corrosion and Electrodeposition. Final rept., J. Kruger. 1982, 19p
Pub. in Proceedings of Diagrams of Chemical and Electrochemical Equilibria: Their Setting-Up and Applications, Brussels, Belgium, September 2-5, 1981, p215-233 1982.

Keywords: *Chemical equilibrium, *Corrosion prevention, *Electrodeposition, *Phase diagrams, Passivity, pH, Electrolysis, Oxidation, Reviews, Metal coatings, Solutions.

The application of the equilibrium pH-potential diagrams to corrosion has been a crowning accomplishment of CEBELCOR, especially its founder, M. Pourbaix. This review will describe the application of these diagrams to both corrosion and electrodeposition problems in aqueous systems at room temperature. For corrosion the diagrams have been used in the classic applications of establishing theoretical domains of conditions for corrosion, immunity and passivation, resistance of metals to pure water, the use of oxidizing corrosion inhibitors, and the classification of the degree of nobility of metals. Other applications have been to localized corrosion, passivity, problems in complex practical environments, e.g., atmospheric corrosion, useful corrosion processes and corrosion protection measures. For electrodeposition, the diagrams have been used to determine conditions to promote desired cathodic and anodic processes and to select suitable electrolytic solutions. The application of the diagrams to the development of new electrodeposition technologies, e.g., pulsed electrodeposition of alloy coatings, looks promising.

500,406
PB86-111838 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Inorganic Materials Div.
Passivity and Breakdown of Passivity. Final rept., J. Kruger. 1982, 14p
Sponsored by Office of Naval Research, Arlington, VA.
Pub. in Proceedings of Electrochemistry in Industry: New Directions, Cleveland, OH., October 20-22, 1980 p317-330 1982.

Keywords: *Passivity, *Corrosion, *Iron, *Surface chemistry, Electrochemistry, Ferrochromium, Molecular structure, Films.

The structure, composition and mechanism of formation of the passive film on iron is described. Breakdown of passivity mechanisms are discussed along with the role that structure and alloy composition play in breakdown processes.

500,407
PB86-111861 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.
Structure of Passive Films on Iron Using a New Surface-EXAFS (Extended X-ray Absorption Fine Structure) Technique. Final rept., G. G. Long, J. Kruger, D. R. Black, and M. Kuriyama. 1983, 8p
Pub. in Jnl. of Electroanalytical Chemistry and Interfacial Electrochemistry 150, n1-2 p603-610 1983.

Field 7—CHEMISTRY

Group 7D—Physical Chemistry

Keywords: *Molecular structure, *Surface chemistry, *Iron, *Iron oxides, *Corrosion, Chemical bonds, Crystal structure, Fine structure, Reprints, *Extended X ray absorption fine structure.

There exists considerable controversy about the structure, the bonding, and the composition of the passive films that form on iron surfaces in aqueous electrolytes. A major problem is that most of the surface analytical techniques used to characterize the passive film require exposure to vacua, which can alter the structure of the passive film. This study seeks to overcome this problem through the application of a new surface-EXAFS (extended x-ray absorption fine structure) technique that is both extremely sensitive to structural and bonding changes in the 2 to 3 nm passive film and does not require the use of a vacuum environment. Near edge and extended x-ray absorption fine structure spectra from passive films on iron were measured and compared with those from pure iron and a polycrystalline iron oxide of known structure. The EXAFS data provide a measure of the relative disorder in the passive films, and they were used to derive bond lengths for the iron-to-oxygen and the iron-to-iron coordination shells.

500,408

PB86-111911 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.

Adsorption and Decomposition of N₂O on Ru(001).
Final rept.,
T. E. Madey, N. R. Avery, A. B. Anton, B. H. Toby, and W. H. Weinberg. 1983, 2p
Pub. in Jnl. of Vacuum Science and Technology, A1 n2 p1220-1221 Apr/Jun 83.

Keywords: *Nitrogen oxide(N₂O), *Adsorption, *Decomposition, *Surface chemistry, Chemisorption, Chemical bonds, Ruthenium, Reprints, Molecular configuration.

The authors found evidence that N₂O binds to Ru(001) at 75K via the N atom in both vertical and inclined configurations, and that chemisorbed N₂O both desorbs molecularly and decomposes to N₂(g) and O(ads) when the surface is heated.

500,409

PB86-111929 Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.

Nascent Vibrational and Rotational Distributions from the Charge Transfer Reaction Ar(+1) + CO yields CO(+1) + Ar at Near Thermal Energy.
Final rept.,
G. H. Lin, J. Maier, and S. R. Leone. Jun 85, 9p
Grants NSF-CHE79-11340, NSF-PHY82-00805
Sponsored by National Science Foundation, Washington, DC.
Pub. in Jnl. of Chemical Physics 82, n12 p5527-5535, 15 Jun 85.

Keywords: *Molecular vibrational, *Molecular rotational, Carbon monoxide, Argon, Fluorescence, Reprints, *Laser induced fluorescence, *Flowing afterglow, *Ion molecule collision, Franck-Condon principle, Argon ions.

Saturated laser-induced fluorescence detection is used to study the vibrational and rotational distributions produced in the charge transfer reaction Ar(+1)(doublet + P(sub 3/2)) + CO(X) singlet sigma(+1) nu=0 yields Ar(singlet S(sub 0)) + CO(+1) (X doublet sigma(+1), nu=0-7) at 0.2 eV energy. The apparatus combines a flowing afterglow ion source with a sampling orifice to obtain a supersonic expansion of near thermal energy ions for reaction under nearly single collision conditions in the reaction chamber. The experimental results are better explained by a potential surface crossing at close approach, than either by considerations of strict Franck-Condon overlaps or energy resonance.

500,410

PB86-111937 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Inorganic Materials Div.

Steric Effects in Neophytin(IV) Chemistry.
Final rept.,
T. P. Lockhart. 1985, 8p
Pub. in Jnl. of Organometallic Chemistry 287, n2 p179-186 1985.

Keywords: *Nuclear magnetic resonance, Metal containing organic compounds, Stability, Solutions, Chemical

equilibrium, Reprints, *Steric effects, *Distannoxane/neophyl.

The stability and self-association in solution of (neophyl₃Sn)₂O, neophyl₃SnOH, and (neophyl₃Sn)₂CO₃ (neophyl = C₆H₅(CH₃)₂CCH₂) have been examined by ¹¹⁹Sn NMR. The presence of Sn₂Sn spin coupling through oxygen (doublet J(119Sn,117Sn)) has been used to distinguish between the distannoxane and stannol. These observations are in sharp contrast with a previous report that the sterically bulky neophyl ligands render neophyl₃SnOH stable toward dehydration. Singlet J((119)Sn,(13)C) observed for neophyl₃SnOH and (neophyl₃Sn)₂CO₃ indicates that these compounds, unlike their n-alkyl-substituted homologues, are unassociated in solution, a result attributed to the steric bulk of the neophyl ligand.

500,411

PB86-111978 Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.

High Excitation of Two Electrons.
Final rept.,
A. R. P. Rau. 1984, 14p
Grant NSF-PHY81-20243
Sponsored by National Science Foundation, Washington, DC.
Pub. in Proceedings of International Conference on Atomic Physics (9th), Seattle, WA., July 1984, Atomic Physics 9, p491-504.

Keywords: *Atomic energy levels, Excitation, Quantum numbers, Oxygen, *Electron electron interactions.

Doubly-excited states of high excitation in atoms and ions - their description through appropriate quantum numbers, mechanisms for their excitation and very recent experimental evidence for them - are reviewed. The states are divided into two classes depending on whether the two electrons have comparable excitation or are widely disparate in their radial extent. Different sets of quantum numbers are appropriate to the description of the two kinds of states. In particular, the states of high and comparable excitation are best viewed as a single entity, the pair, attached to the grandparent ion, with a reference throughout only to quantum numbers characteristic of the pair. Elements from the literature on planetary atoms, ridge states, O₄ group symmetry for two electrons, the adiabatic hyperspherical method, and the Wannier theory for two-electron escape are brought together in the description of pathways to, and properties of, high excitation.

500,412

PB86-112000 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Thermophysics Div.

Liquid-Vapor Interface of a Binary Liquid Mixture Near the Consolute Point.
Final rept.,
J. W. Schmidt, and M. R. Moldover. 15 Aug 85, 6p
Sponsored by National Aeronautics and Space Administration, Washington, DC.
Pub. in Jnl. of Chemical Physics 83, n4 p1829-1834, 15 Aug 85.

Keywords: *Surface chemistry, *Binary systems(Materials), *Critical point, Polarimetry, Molecular structure, Mixtures, Ternary systems, Refractivity, Adsorption, Liquid phases, Vapor phases, Temperature, Reprints, *Isopropyl alcohol, *Cyclohexane/fluoro-methyl.

The liquid-vapor interface above mixtures of isopropanol (i-C₃H₇OH) and perfluoromethylcyclohexane (C₇F₁₄) has been studied in the vicinity of the consolute point T(sub c) = 363 K. As three-phase coexistence is approached, the excess fluorocarbon adsorbed at this interface increases; the adsorption is expected to diverge at T(sub c) for a mixture of the critical composition. A simple model of the interface which incorporates the adsorption anomaly is compared with out ellipticity measurements. Both the model and our data yield ellipticities which have a finite maximum at 0.1 K above T(sub c). Ellipticity data for noncritical compositions are presented; however, their analysis will be presented elsewhere.

500,413

PB86-112018 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.

Oxygen-Induced CO Reorientation on Cr(110).

Final rept.,
N. D. Shinn, and T. E. Madey. Jun 85, 5p
Sponsored by Department of Energy, Washington, DC.
Pub. in Jnl. of Vacuum Science and Technology A3, n3 p1673-1677 May/Jun 85.

Keywords: *Carbon monoxide, *Chemisorption, *Oxygen, Chromium, Surface chemistry, Chemical bonds, Reprints, Electron energy loss spectroscopy, Electron stimulated desorption ion angular distributions, Low energy electron diffraction, Auger electron spectroscopy.

Studies of CO and CO/O chemisorption on Cr(110) at 120 K using high resolution electron energy loss spectroscopy (EELS), electron stimulated desorption ion angular distributions (ESDIAD), low energy electron diffraction (LEED), and Auger electron spectroscopy (AES) are reported. On the clean surface, two molecular binding modes are sequentially populated.

500,414

PB86-112034 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Inorganic Analytical Research Div.

Further Developments in the High-Precision Coulometric Titration of Uranium.
Final rept.,
T. Tanaka, G. Marinenko, and W. F. Koch. 1985, 6p
Pub. in Talanta 32, n7 p525-530 1985.

Keywords: *Uranium, *Chemical analysis, *Volumetric analysis, *Coulometers, Experimental design, Performance evaluation, Reprints.

An experimental study of the current efficiency in the coulometric generation of Ti(III), as a function of electrolyte composition, current density and electrode material, has been performed. The cathodes investigated include platinum, mercury and graphite. The first two are suitable for high-precision determination of uranium. The graphite surface is readily poisoned, rendering it useless for high-accuracy work. The use of mercury requires thorough removal of chloride from the system. The precision and error obtained are comparable for both the mercury and platinum cathodes, and are of the order of 50 ppm.

500,415

PB86-112042 Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.

Two-Laser Pulse-and-Probe Study of T-R,V Energy Transfer Collisions of H + NO at 0.95 and 2.2 eV.
Final rept.,
C. A. Wight, D. J. Donaldson, and S. R. Leone. 15 Jul 85, 8p
Sponsored by Army Research Office, Research Triangle Park, NC.
Pub. in Jnl. of Chemical Physics 83, n2 p660-667, 15 Jul 85.

Keywords: *Molecular rotation, *Molecular vibration, *Spin orbit interactions, Nitrogen oxide(NO), Excitation, Temperature, Reprints, *Atom molecule collision, *Laser induced fluorescence, Hydrogen atoms.

Vibrational, rotational, and spin-orbit state distributions are obtained for inelastic collisions of H+NO at 2.2 and 0.95 eV. The H atoms are generated by excimer laser photolysis of H₂S at 193 and 248 nm, respectively, and the excited states of the NO molecules are probed by laser-induced fluorescence using a tunable dye laser. The rotational state distribution accompanying the T-V excitation of nu = 1-3 at 2.2 eV is approximately characterized by a Boltzmann distribution at 1275 K, and is essentially independent of the vibrational level excited. At 0.95 eV, the rotational populations are approximately characterized by a 1050 K distribution. In each case, the temperatures of the spin-orbit state populations and the rotational states are the same. No selective population of lambda doublet states is observed. The results are discussed in terms of chemical interactions between these two open-shell species on the HNO potential energy surfaces.

500,416

PB86-112091 Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.

Multiple Ionization of a Hartree Atom by Intense Laser Pulses.

Final rept.,
S. Geltman. 29 Apr 85, 4p
Pub. in *Physical Review Letters* 54, n17 p1909-1912, 29 Apr 85.

Keywords: *Ionization, *Hartree-Fock approximation, *Atoms, Atomic orbitals, Reprints, *Laser applications.

It is shown that a good representation of recent experimental results on the relative production of multiply charged ionic states by intense laser pulses of various wavelengths may be obtained on the basis of Hartree's independent-electron shell model of the atom.

500,417

PB86-112109 Not available NTIS
National Bureau of Standards (NML), Boulder, CO.
Quantum Physics Div.

Dielectronic Recombination as a Direct Free-Bond Radiative Process.

Final rept.,
S. Geltman. 1985, 18p
Grant NSF-PHY82-00805
Sponsored by National Science Foundation, Washington, DC.
Pub. in *Jnl. of Physics B: Atomic and Molecular Physics* 18, n7 p1425-1442 1985.

Keywords: *Atomic energy levels, Ionization, Chemical equilibrium, Elastic scattering, Comparison, Excitation, Reprints, *Autoionization, *Dielectronic recombination, *Dipole radiation, Electron ion collision, Rydberg series.

The process of dielectronic recombination is studied in terms of the standard treatment of a free-bound dipole radiative transition between stationary states. The initial free state of electron-ion resonant elastic scattering is analysed using the Fano formulation for discrete-state-continuum configuration mixing. In most cases there is reasonable overall qualitative agreement, but uncertainties in the final-state distributions involved in the measurements prevent a fully quantitative comparison. The effects of external fields on the dielectronic recombination process are also discussed in the context of the present method.

500,418

PB86-112141 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Inorganic Analytical Research Div.

High Sensitivity Neutron Activation Analysis of Environmental and Biological Standard Reference Materials.

Final rept.,
R. R. Greenberg, R. F. Fleming, and R. Zeisler. 1984, 8p
Pub. in *Environment International* 10, p129-136 1984.

Keywords: *Neutron activation analysis, *Environmental surveys, Chemical analysis, Sampling, Trace elements, Laboratory equipment, Reprints, *Standard reference materials, *Biological processes.

Neutron activation analysis is a sensitive method with unique capabilities for the analysis of environmental and biological samples. Since it is based upon the nuclear properties of the elements, it does not suffer from many of the chemical effects that plague other methods of analysis. Analyses can be performed either with no chemical treatment of the sample (instrumentally), or with separations of the elements of interest after neutron irradiation (radiochemically). Typical examples of both types of analysis are discussed, and data obtained for a number of environmental and biological SRMs are presented.

500,419

PB86-112158 Not available NTIS
National Bureau of Standards (NML), Boulder, CO.
Quantum Physics Div.

Product Vibrational State Distributions of Thermal Energy Charge Transfer Reactions Determined by Laser-Induced Fluorescence: $N(+1) + CO$ yields $CO(+1)(\nu=0-2) + N$.

Final rept.,
C. E. Hamilton, V. M. Bierbaum, and S. R. Leone. Jul 85, 10p
Sponsored by Air Force Office of Scientific Research, Bolling AFB, DC.
Pub. in *Jnl. of Chemical Physics* 83, n2 p601-610, 15 Jul 85.

Keywords: *Molecular vibration, Carbon monoxide, Nitrogen, Dynamics, Reprints, *Laser induced fluores-

cence, *Ion molecule interactions, *Flowing afterglow, Nitrogen ion.

The nascent vibrational state distribution of the $N(+1) + CO$ yields $CO(+1)(\nu=0-2) + N$ charge transfer reaction is measured at thermal energy. The reaction is carried out in a flowing afterglow and the vibrational state populations are determined by laser-induced fluorescence on the $CO(+1)(A(\text{sup } 2) \pi-X(\text{sup } 2) \sigma(+1))$ system. The observed vibrational distribution suggests that neither a long-range Franck-Condon mechanism nor an energy resonant process adequately describes the charge transfer reaction. A dual channel mechanism of the reaction is considered, in which a fraction of the reactive collisions proceed by a long-range Franck-Condon mechanism while the remainder proceed via a long-lived $NCO(+1)$ intermediate. The intermediate may lead to the observed extent of $CO(+1)$ vibrational excitation either through statistical partitioning of the energy or by dynamical changes in the CO bond length through specific molecular orbital occupancies.

500,420

PB86-112166 Not available NTIS
National Bureau of Standards (NML), Boulder, CO.
Quantum Physics Div.

Nascent Product Vibrational State Distributions of Thermal Ion-Molecule Reactions Determined by Infrared Chemiluminescence.

Final rept.,
C. E. Hamilton, and S. R. Leone. 1985, 18p
Grant NSF-PHY82-00805
Sponsored by National Science Foundation, Washington, DC., and Air Force Office of Scientific Research, Bolling AFB, DC.
Pub. in *Gas Phase Chemiluminescence and Chemiluminescence*, p139-156 1985.

Keywords: *Molecular vibration, *Infrared analysis, *Chemiluminescence, Excitation, Chemical reactions, Reprints, *Ion molecule interactions, *Flowing afterglow.

A flowing afterglow apparatus is used to study the dynamics of ion-molecule reactions by detection of vibrational states in the products with infrared chemiluminescence. Other reactions of polyatomic molecules have been studied to test whether the products are formed in a 'direct' fashion or through a long-lived collision intermediate. The results are compared to successful theoretical models of Gauyacq, in which the electron is released by dynamically-induced transitions on the outer region of the potential upon the initial reagent approach.

500,421

PB86-112174 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Molecular Spectroscopy Div.

Temperature Dependence of the Vibrational Population Lifetime of $OH(\nu=1)$ in Fused Silica.

Final rept.,
E. J. Heilweil, M. P. Casassa, R. R. Cavanagh, and J. C. Stephenson. 7 Jun 85, 6p
Sponsored by Air Force Office of Scientific Research, Bolling AFB, DC.
Pub. in *Chemical Physics Letters* 117, n2 p185-190, 7 Jun 85.

Keywords: *Silicon dioxide, *Molecular vibration, *Infrared spectroscopy, *Relaxation(Mechanics), Reprints, *Hydroxyl radicals, *Picosecond pulses.

An infrared picosecond transient bleaching technique was used to measure vibrational lifetimes $T(\text{sub } 1)$ of hydroxyl groups in fused silica over the temperature range 100-1450 K. $T(\text{sub } 1)$ decreases from 109 to 15 ps in this range. The $T(\text{sub } 1)$ temperature dependence is compared to non-radiative relaxation theory for the decay of the $OH(\nu=1)$ quantum by a multiphonon mechanism.

500,422

PB86-112745 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.

Beam Broadening in a Strongly Scattering Target in the Analytical Electron Microscope.

Final rept.,
A. D. Romig, D. E. Newbury, and R. L. Myklebust. 1982, 5p
See also DE82-014085. Sponsored by Microbeam Analysis Society, Bethesda, MD.
Pub. in *Proceedings of Annual Conference on Microbeam Analysis Society* (17th), Washington, DC., August 9-13, 1982, p88-92.

Keywords: *Electron microscopy, *Electron scattering, *Uranium alloys, *X ray analysis, Experimental design, Beam width, Chemical analysis, Monte Carlo method.

Beam broadening has been studied in alloys of uranium-niobium and uranium-molybdenum. Profiles have been measured across interphase boundaries for which the solute element is located exclusively in one phase. Experimental measurements have been compared with calculated profiles obtained with a Monte Carlo electron trajectory simulation. Good agreement is obtained in the immediate region of the boundary. A long low intensity tail is indicated from the calculations but this tail is not observed experimentally. Studies of the effect of varying specimen and beam parameters indicate the difficulty in obtaining accurate experimental profiles.

500,423

PB86-112828 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.

Chemisorbed Oxygen on Ni(110) Studied by Spin Polarized Inverse Photoemission.

Final rept.,
C. S. Feigerle, A. Seiler, J. L. Pena, R. J. Celotta, and D. T. Pierce. 1985, 4p
Sponsored by Office of Naval Research, Arlington, VA., and National Science Foundation, Washington, DC.
Pub. in *Jnl. of Vacuum Science and Technology*, A3 n3 p1487-1490 May/Jun 85.

Keywords: *Chemisorption, *Oxygen, *Surface chemistry, *Oxidation, Nickel, Polarization(Spin alignment), Electron diffraction analysis, Reprints, *Spin polarized inverse photoemission spectroscopy, Low energy electron diffraction, Auger electron spectroscopy.

Dissociative chemisorption of O_2 on the surface on Ni(110) has been investigated by the techniques of AES, LEED, and spin polarized inverse photoemission spectroscopy (SPIES). SPIES provides a unique method for studying the empty electronic states of the majority and minority spin bands separately and at the same time serves as a surface magnetometer. This is taken as evidence for interactions of the adsorbate with the d levels of the substrate.

500,424

PB86-112844 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.

Interfacially Controlled Phenomena in the System Potassium Carbonate-Potassium Aluminate.

Final rept.,
L. P. Cook. 1981, 12p
Sponsored by Department of Energy, Washington, DC.
Pub. in *Materials Science Research* 14, p143-154 1981.

Keywords: *Potassium carbonates, *Potassium aluminates, *Interfacial tension, Melting points, Crystallography, Liquid phases, Experimental design, Reprints, Clathrate compounds.

Anomalous melting behavior is described in the system K_2CO_3 -KA102. Compositions with less than 90 mole % K_2CO_3 show no evidence of melting at 1150C despite the known melting of pure K_2CO_3 at 901C. X-ray analysis of the products shows primarily well-defined patterns of K_2CO_3 and KA102. The influence of platinum reaction and surface tension effects is discussed. The possibility of a regular intergrowth of potassium carbonate with potassium aluminate along a crystallographically-controlled interface at temperatures above the melting point of K_2CO_3 is suggested as a way of explaining the experimental data. This intergrowth could occur either in the form of an intercalation-type solid or as a partially ordered liquid (mesomorphic) phase.

500,425

PB86-112893 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Semiconductor Materials and Processes Div.

Improved Analysis Procedures for Deep-Level Measurements by Transient Capacitance.

Final rept.,
W. E. Phillips, W. R. Thurber, and J. R. Lowney. 1983, 6p
Pub. in *Proceedings of the Electrochemical Society* 83-9, p485-490 1983.

Keywords: *Semiconductor diodes, *Semiconductors(Materials), Semiconductor doping,

Field 7—CHEMISTRY

Group 7D—Physical Chemistry

Density(Mass/volume), Platinum, Silicon, Reprints, *Deep level transient spectroscopy.

The procedures reported here provide a way to analyze data from nonexponential transient capacitance measurements made under conditions such that (a) the traps are charged in only a part of the depletion layer or (b) the trap density is not small compared with the net shallow dopant density. This analysis requires $1/(C \text{ squared})$ vs. V data to be linear over the voltage range used, which may be a small range at low temperatures because of the compensation effect of traps. Computer simulations of $1/(C \text{ squared})$ vs. V plots are given for various ratios of trap and dopant densities at several temperatures and show ranges which are sufficiently linear, but which have a trap-density-dependent slope. These effects are illustrated by experimental $1/(C \text{ squared})$ vs. V , isothermal transient capacitance (ITCAP), and DLTS measurements for a wide range of densities of platinum in $p(\text{sup } +)n$ and $n(\text{sup } +)p$ silicon diodes.

500,426
PB86-113636 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Inorganic Materials Div.
Defects and Charge Transport in Stabilized α -Ta₂O₅.

Final rept.,
A. McHale, and H. L. Tuller. Aug 83, 15p
Pub. in Radiation Effects 75, n1-4 p267-281 Aug 83.

Keywords: *Tantalum oxide, *High temperature tests, Stability, Electronic conductivity, Transport properties, Ions, Thermodynamics, Reprints.

The high temperature form of tantalum oxide, α -Ta₂O₅, stabilized by the addition of several mol% Sc₂O₃ has been shown to be an excellent oxygen conductor, comparable to stabilized zirconias in the range 500-950°C. Electrical conductivity is characterized by the dominant ionic component in air, with an activation ene of about/ev. N-type electronic conduction, proportional to $P(\text{sub } O_2)(\text{sup } -1/4)$, becomes significant at highly reduced oxygen partial pressures and high temperatures. Transport properties have been characterized using complex impedance methods. Galvanic cell measurement of ionic transference number was used to confirm oxygen ions as dominant charge carriers. Both polycrystalline and single crystal specimens were examined. Stabilization of high Ta₂O₅ via incorporation of aliovalent impurities is discussed in relation to its probable effects on crystalline anisotropy and charge transport.

500,427
PB86-113693 PC A03/MF A01
National Bureau of Standards (NML), Gaithersburg, MD. Office of Standard Reference Materials.
Development of a One-Micrometer-Diameter Particle Size Standard, SRM (Standard Reference Materials) 1690.

Final rept.,
G. W. Mulholland, A. W. Hartman, G. G. Hembree, E. Marx, and T. R. Lettieri. May 85, 36p NBS/SP-260/95
Also available from Supt. of Docs as SN003-003-02665-4. Library of Congress catalog card no. 85-600539.

Keywords: *Particle size, *Standards, *Particle size distribution, Refractivity, Aerosols, Light scattering, Polystyrene, Spheres, Error analysis, *Standard reference materials, Transmission electron microscopy.

The average diameter of the first micrometer particle size standard (Standard Reference Material 1690), an aqueous suspension of monosized polystyrene spheres with a nominal 1micrometers diameter, was accurately determined by three independent techniques. In one technique the intensity of light scattered by a diluted suspension of polystyrene spheres was measured as a function of scattering angle, using a He-Ne laser polarized in the vertical direction. The second technique consisted of measuring the intensity of light scattered from individual polystyrene spheres suspended in air as a function of angle, using a He-Cd laser with light polarized parallel and perpendicular to the scattering plane. The measurement of row length by optical microscopy for polystyrene spheres arranged in close-packed, two-dimensional hexagonal arrays was the basis of the third technique. The measurement errors for each technique were quantitatively assessed.

500,428
PB86-114063 Not available NTIS

National Bureau of Standards, Gaithersburg, MD.
Analysis and Modeling of the Leaching Process.

Final rept.,
R. C. Paule. 1981, 24p
Sponsored by American Society for Testing and Materials, Philadelphia, PA.
Proceedings of Conference on Hazardous Solid Waste Testing (1st), Fort Lauderdale, FL, January 14-15, 1981, ASTM STP 760, p112-135 1981.

Keywords: *Fly ash, *Leaching, *Extraction, *Environmental surveys, *Hazardous materials, Chemical equilibrium, Statistical analysis, Chemical analysis, Solid wastes.

A statistical analysis has been made on data obtained in the study of the leaching process for the ASTM special fly ash sample using distilled water as the extractant. Two laboratories made extractions under a variety of conditions, and after acid stabilization, the leachates were analyzed by a third laboratory using ICP analysis. Fifteen elements were studied. Three types of experimental variables were examined: (1) the extractor (60 and 180 cycle/minute shaker tables, and the NBS mixer), (2) the liquid/solid ratio (4/1, 10/1, and 20/1), and (3) the time (24 and 48 hours). The data were examined in terms of three plausible extraction models.

500,429
PB86-119229 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Inorganic Materials Div.
Studies of Passive Film Breakdown by Detection and Analysis of Electrochemical Noise.

Final rept.,
U. Bertocci, and J. Kruger. 1980, 11p
Pub. in Surface Science 101, n1-3 p608-618 1980.

Keywords: *Electric current, *Electrodes, *Electrochemistry, *Acoustic measurement, Passivity, Corrosion, Aluminum, Amorphous alloys, Surface chemistry, Reprints, *Passivation(Semiconductor), *Noise exposures.

Random fluctuations in the passive current of electrodes under potentiostatic conditions have been measured on aluminum in boric acid: borate solution and on a Fe-Cr-Ni alloy, both in the amorphous and in the crystalline state, in sulfuric acid. The onset of pitting can be detected by the large increase in current noise. The noise level is different in the amorphous and crystalline Fe-Cr-Ni alloy, indicating that the breakdown of the passive film differs in the two conditions. The experimental aspects involved in carrying out meaningful noise measurements in electrochemical systems are also discussed.

500,430
PB86-119237 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD.
Martensitic Transformations in Iron-Nickel-Carbon Alloys.

Final rept.,
T. N. Durlu, and J. W. Christian. 1979, 6p
Pub. in Proceedings of International Conference on Martensitic Transformations (ICOMAT), Cambridge, MA., June 24-29, 1979, p343-348.

Keywords: *Phase transformation, *Crystallography, *Martensite, Reaction kinetics, Stress strain analysis, *Iron nickel carbides.

Small austenitic single crystals of two alloys with sub-zero $M(\text{sub } s)$ (burst) temperatures were spark-machined from recrystallized samples and used in both the undeformed and deformed conditions to investigate the subsequent transformation. The $M(\text{sub } s)$ temperature as a function of reduction in area by rolling increased to a broad maximum at 40-50% deformation and then decreased again. Crystallographic investigations were made of the preferred habit plane variants formed in the first burst in single crystals of many different orientations predeformed in compression. Most of the crystals were orientated for single slip and the initial transformation occurred by the co-operative formation of a single group of plates with four habit plane variants. It is believed that the results indicate that an active slip system stimulates particular habit plane variants rather than inhibits others. Studies were also made of deformation-induced martensite in polycrystalline samples of Fe-Ni-C alloys. Different morphologies were found for stress-induced and strain-induced martensites.

500,431
PB86-119294 Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Time and Frequency Div.

Far-Infrared Laser Magnetic Resonance Spectrum of the SiH Radical and Determination of Ground State Parameters.

Final rept.,
J. M. Brown, R. F. Curl, and K. M. Evenson. 1984, 7p
Sponsored by National Aeronautics and Space Administration, Washington, DC.
Pub. in Jnl. of Chemical Physics 81, n7 p2884-2890, 1 Oct 84.

Keywords: *Molecular energy levels, *Silane, Free radicals, Reprints, *Laser spectroscopy, *Far infrared laser magnetic resonance spectroscopy.

The far-infrared laser magnetic resonance (LMR) spectrum of the SiH radical in the $\nu=0$ level of its X (sup 2)pi state has been recorded. The signals are rather weak. The molecules were generated in the reaction between fluorine atoms and SiH₄. Rotational transitions have been detected in both (sup 2)pi(sub 1/2) and (sub 2)pi(sub 3/2) spin components but no fine structure transitions between the spin components were observed. Proton hyperfine splittings were resolved on some lines. The measurements have been analyzed, subjected to a least-squares fit using an effective Hamiltonian and the appropriate molecular parameters determined. The weakness of the spectrum and the failure of attempts to power saturate favorable lines are both consistent with a small value for the electric dipole moment for SiH.

500,432
PB86-119302 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD.
Modeling of Axially Symmetric Flow Reactors.

Final rept.,
R. L. Brown. 1984, 7p
Pub. in Computers and Chemistry 8, n2 p139-145 1984.

Keywords: *Mathematical models, *Axisymmetric flow, *Chemical reactors, Reaction kinetics, Velocity measurement, Concentration(Composition), Reprints.

A method of calculating the velocity profiles and species concentrations in axially symmetric flow reactors is presented. The method is illustrated with a reactor consisting of three concentric tubes arranged so that reactants flow through the inner tube and inner annulus to a mixing region and the products flow out through the outer annulus. A single bimolecular reaction is used in the example. The method involves two steps; calculation of the velocity field from a solution of the Navier-Stokes equations, followed by solution of the species conservation equations. The technique provides a way of analyzing reactors with variable cross sections and sampling ports near mixing regions.

500,433
PB86-119336 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD.
Studies of Internal Interfaces in Solid Electrolytes by Impedance Spectroscopy.

Final rept.,
C. K. Chiang, A. L. Dragoo, and A. D. Franklin. 1981, 1p
Pub. in Jnl. of the Electrochemical Society 128, n3 p124C 1981.

Keywords: *Electrodes, *Solid electrolytes, *Electrical impedance, *Spectrographic analysis, Ceramics, Crystals, Interfaces, Surface chemistry, Additives, Electrochemistry, Grain boundaries, Reprints, Cesium oxides, Lanthanum chromites, Yttrium chromates.

The frequency dependence of the impedance of the system electrode/solid electrolyte/electrode contains information about charge transport processes not only at the solid electrolyte/electrode interfaces and within the single-crystal grains of the solid electrolyte itself, but also at internal interfaces within the solid and Ca-doped γ -CrO₃ illustrate how grain-boundaries may be studied.

500,434
PB86-119377 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.

Orientalional Ordering in a Strongly Chemisorbed System: Na on Ru(001).

Final rept.,
D. L. Doering, and S. Semancik. 1984, 4p
Sponsored by Department of Energy, Washington, DC.
Pub. in Physical Review Letters 53, n1 p66-69, 2 Jul 84.

Keywords: *Sodium, *Surface chemistry, *Chemisorption, *Crystal structure, Rhuthenium, Substrates, Mathematical models, Rare gases, Orientation, Reprints, *Low energy electron diffraction.

The study of Na on Ru(001) at 80 K provides the first detailed examination of orientational ordering in a strongly chemisorbed monolayer. The relative orientation of a Na layer on Ru(001) varies with the Na-Ru lattice misfit in a way consistent with predictions from theoretical models that have been used to explain orientational ordering of rare gases physisorbed on graphite. The similarity between physisorbed systems and the chemisorbed Na on Ru system suggests a universal behavior of rigid overlayers on hexagonal substrates.

500,435

PB86-119385

Not available NTIS

National Bureau of Standards (NML), Gaithersburg, MD.

Structure of the 1:1 Molecular Complex of Pyrene and Dicyanomethylenecroconate.

Final rept.,
R. M. Doherty, J. M. Stewart, A. D. Mighell, C. R. Hubbard, and A. J. Fatiadi. 1982, 5p
Pub. in Acta Crystallographica, Section B: Structural Crystallography and Crystal Chemistry, B38 n3 p859-863 1982.

Keywords: *Complex compounds, *Crystal structure, *X ray diffraction, Reprints, *Pyrene, *Cyclopentene dione/dicyanomethylene-diethoxy.

A 1:1 molecular complex of pyrene and 2-dicyanomethylene-4,5-diethoxy-4-cyclopentene-1,3-dione (DDC) is formed upon evaporation of a solution containing equimolar amounts of the two substances. The product is a charge-transfer complex containing a novel oxocarbon acceptor. The crystal structure of the adduct has been determined by single crystal x-ray diffraction.

500,436

PB86-119443

Not available NTIS

National Bureau of Standards (NEL), Boulder, CO. Chemical Engineering Science Div.

Isochoric (p, V(sub m), x, T) Measurements on (Methane + Ethane) from 100 to 320 K at Pressures to 35 MPa.

Final rept.,
W. M. Haynes, R. D. McCarty, B. E. Eaton, and J. C. Holste. 1985, 24p
Sponsored by Gas Research Inst., Chicago, IL.
Pub. in Jnl. of Chemical Thermodynamics 17, p209-232 1985.

Keywords: *Methane, *Ethane, *Thermodynamics, Mixture, Density(Mass/volume), Equations of state, Comparison, Pressure, Volume, Temperature, Reprints, *Isochore, Corresponding states models, Benedict-Webb-Rubin equation.

Comprehensive isochoric (p, V(sub m), x, T) values have been obtained for (xCH₄+(1-x)C₂H₆) with x=0.35, 0.50, and 0.69 at amount-of-substance densities from 1 to 25 mol/cu dm. The measurements for each composition cover a temperature range from approximately 100 to 320 K at pressures up to 35 MPa. For each mixture the results have been fit to a 32-term modified Benedict-Webb-Rubin equation of state. Further development of the extended corresponding-states model has been accomplished using the results presented here. Comparisons with values from independent sources have been made where possible.

500,437

PB86-119450

Not available NTIS

National Bureau of Standards (NEL), Boulder, CO. Chemical Engineering Science Div.

Orthobaric Liquid Densities and Dielectric Constants of Ethylene.

Final rept.,
W. M. Haynes. 1985, 3p
Pub. in Cryogenics 25, p68-70 1985.

Keywords: *Ethylene, *Dielectric properties, *Density(Mass/volume), Temperatures, Comparison,

Reprints, *Orthobaric liquids, Clausius Mossotti function.

Measurements of the orthobaric liquid densities and dielectric constants of ethylene have been obtained at temperatures from 200 to 270 K. Simultaneous measurements of these properties were carried out using a magnetic suspension densimeter and a concentric cylinder capacitor. Comprehensive comparisons of the present results with the data of other investigators are presented. Also reported are computed values of the Clausius-Mossotti function.

500,438

PB86-119468

Not available NTIS

National Bureau of Standards (NEL), Gaithersburg, MD. Thermophysics Div.

Critical-Point Conditions for Classical Polydisperse Fluids.

Final rept.,
K. A. Johnson, D. A. Jonah, J. M. Kincaid, and G. Morrison. 1985, 6p
Sponsored by Department of Energy, Washington, DC. Office of Basic Energy Sciences.
Pub. in Jnl. of Chemical Physics 82, n11 p5178-5183, 1 Jun 85.

Keywords: *Critical point, *Fluids, Density(Mass/volume), Temperature, Chemical composition, Gibbs free energy, Dispersion, Reprints.

The critical-point conditions for a polydisperse mixture are shown to be equivalent to those for the existence of nontrivial solutions to two homogeneous integral equations of the Fredholm type. This mathematically rigorous treatment is not dependent on the form of any particular model free energy and hence shows that there is no formal distinction between the critical-point conditions of a polydisperse fluid and those conditions derived by Gibbs for the critical point of a mixture with a finite number of components. Using the method of Fredholm, the authors express the critical-point conditions in terms of the zeros of two absolutely convergent expansions, and demonstrate how the expansions may be used to determine the shifts in critical density and temperature caused by changes in the composition of the fluid.

500,439

PB86-122835

Not available NTIS

National Bureau of Standards, Gaithersburg, MD. Inorganic Materials Div.

Structural Investigations by Solid-State (sup 13)C NMR. Dependence of (singlet J((sup 119)Sn, (sup 13)C)) on the Me-Sn-Me Angle in Methyltin(IV)s.

Final rept.,
T. P. Lockhart, W. F. Manders, and J. J. Zuckerman. 1985, 2p
Sponsored by Office of Naval Research, Arlington, VA. Pub. in Jnl. of the American Chemical Society 107, p4546-4547 1985.

Keywords: *Molecular structure, *Isotopic labeling, *Nuclear magnetic resonance, Molecular energy levels, Reprints, Solid state chemistry, Stannane/methyl.

The magnitude of (sup 119)Sn,(sup 13)C, 1J₁, has been determined for 13 methyltin solids by ¹³C cross polarization magic angle spinning solid state NMR. The relationship of 1J₁ to the tin coordination number is discussed. The use of the empirical plot for determining the Me-Sn-Me bond angle in uncharacterized solids and for methyltins in solution is noted.

500,440

PB86-122967

Not available NTIS

National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.

Summary Abstract: Methyl Isocyanide Adsorption on Rh(111).

Final rept.,
S. Semancik, G. L. Haller, and J. T. Yates. 1983, 2p
Pub. in Jnl. of Vacuum Science and Technology A: Vacuum, Surfaces and Films 1, n2 pt2 p1226-1227 Apr/Jun 83.

Keywords: *Adsorption, *Surface chemistry, *Dissociation, Reprints, *Methyl isocyanides, *Electron energy loss spectroscopy, *Auger spectroscopy.

High resolution electron energy loss spectroscopy, temperature programmed desorption and Auger electron spectroscopy have been used to characterize the interaction of methyl isocyanide with Rh(111). Thermally-induced changes in the overlayer as well as the effects of preadsorbates have also been considered.

500,441

PB86-123023

Not available NTIS

National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.

Electron- and Photo-Stimulated Desorption of Condensed Molecular Films: Relevance to the Mechanisms of Ion Formation and Desorption.

Final rept.,
R. Stockbauer, E. Bertel, and T. E. Madey. 1983, 2p
Pub. in Jnl. of Vacuum Science and Technology A1, n2 pt2 p1162-1163 Apr/Jun 83.

Keywords: *Ionization, *Desorption, *Monomolecular films, Comparison, Methyl alcohol, Cyclohexane, Hydrogen, Water, Chemical bonds, Surface chemistry, Reprints, *Electron stimulated desorption, *Photon stimulated desorption, *Chemical reaction mechanisms.

Electron and photon stimulated desorption (ESD,PSD) have been applied mainly to adsorbed monolayers and ionic solids. In an attempt to clarify mechanisms of ion deexcitation and desorption in covalent systems we compare ESD of condensed films of hydrogen-bonded methanol (CH₃OH) and water, and non-hydrogen-bonded cyclohexane (C₆H₁₂). There are striking differences in the results. These results are qualitatively consistent with a model by which more massive ions are preferentially neutralized close to the metal surface. The reneutralization rate decreases with increasing film thickness causing an increased yield of higher mass fragments. It appears that the hydrogen-bonding in the methanol layer provides an effective de-excitation mechanism for higher mass fragments at all thicknesses.

500,442

PB86-123064

Not available NTIS

National Bureau of Standards, Gaithersburg, MD. Polymer Science and Standards Div.

C(sup 13) NMR in Oriented Polymers.

Final rept.,
D. L. VanderHart, G. G. A. Boehm, and V. D. Mochel. 1982, 1p
Pub. in Proceedings of International Union of Pure and Applied Chemistry Macromolecular Symposium (28th), Amherst, MA., July 12-16, 1982, p4.

Keywords: *Nuclear magnetic resonance, *Isotopic labeling, *Polymers, *Orientation, *Polyethylene, *Polyethylene terephthalate, Solids, Molecular flow.

The ¹³C solid-state NMR spectra of oriented polymers are useful for investigating orientation and anisotropic molecular mobility. In favorable cases, e.g., polyethylene, the orientation of the non-crystalline regions can be determined. The mobility of crystalline chains in both linear polyethylene and polyethyleneterephthalate will also be discussed.

500,443

PB86-123106

Not available NTIS

National Bureau of Standards (NML), Gaithersburg, MD. Office of Standard Reference Materials.

Reference Data for Thermophysical Properties.

Final rept.,
H. J. White, and J. R. Rumble. 1982, 4p
Pub. in Proceedings of Symposium on Thermophysical Properties, Gaithersburg, MD., June 15-18, 1981, Thermophysical Properties of Solids and of Selected Fluids for Energy Technology 2, p415-418 1982.

Keywords: *Thermophysical properties, *Materials test, Transport properties, Thermodynamics, Physical properties, Crystal structure, Phase diagrams, Sources, *Reference materials.

The activities of the Office of Standard Reference Data of the National Bureau of Standards and the National Standard Reference Data System (NSRDS) for which it provides program management will be discussed briefly. Emphasis will be placed on those activities thought to produce products of interest to workers in the area of thermophysical properties. Included will be data centers and projects covering such technical areas as thermodynamics, transport properties, physical properties, and materials properties such as phase diagrams and crystal structure. An attempt will also be made to list other major sources of evaluated reference data of interest.

500,444

PB86-123130

Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

Field 7—CHEMISTRY

Group 7D—Physical Chemistry

Reliable Data for Flue Gas Desulfurization Processes.

Final rept.,
B. R. Staples. 1982, 16p
Sponsored by American Chemical Society, Washington, DC.
Pub. in Proceedings of Meeting of the American Chemical Society Flue Gas Desulfurization, Atlanta, GA., March 29-30, 1981, p41-56 1982.

Keywords: *Air pollution control equipment, *Scrubbing, *Electrolytes, *Thermodynamic properties, Physical properties, Guidelines, Chemical equilibrium, Enthalpy, Entropy, Performance evaluation, Chemical properties, Flue gases, Specific heat, Gibbs free energy, Activity coefficient, Tables(Data), Flue gas desulfurization.

A wide variety of physical chemical data and vapor liquid equilibria is required to predict and extrapolate performance reliability of flue gas desulfurization processes. A chemical and physical model capable of predicting actual scrubber performance is a continuing goal, but any model is only as reliable as the input data. Carefully evaluated thermodynamic and kinetic data are needed to ensure consistency, accuracy, and to provide a basis for comparing processes or models. The methodology for the critical evaluation of thermodynamic properties of electrolytes is discussed in general, with emphasis on processes important in flue gas washing systems. How we intend to use the present evaluation systems to provide updated data for flue gas washing processes is also discussed. A number of these specific processes was chosen to illustrate the evaluation procedure. Guidelines are provided for calculating an equilibrium constant, activity coefficient, Gibbs energy and enthalpy of reaction, enthalpy of dilution, and standard enthalpy, Gibbs energy, entropy, and heat capacity. Sources of data and how to use them are discussed.

500,445

PB86-123999

Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.

Angular Momentum Transfer and Charge Cloud Alignment in Atomic Collisions: Intuitive Concepts, Experimental Observations and Semiclassical Models.

Final rept.,
I. V. Hertel, H. Schmidt, A. Bahring, and E. Meyer. 1985, 40p
Pub. in Reports on Progress in Physics 48, n3 p375-414 Mar 85.

Keywords: *Angular momentum, Mathematical models, Experimental design, Excitation, Reprints, *Atom atom interactions, *Laser spectroscopy, Sodium atoms, Xenon atoms, Barium atoms.

The authors discuss intuitive concepts to describe alignment and orientation effects in collision processes with, or leading to, an atomic np charge cloud state. For direct excitation one understands the atomic angular momentum transferred to terms of a rolling ball; and for excitation (deexcitation) in a molecular picture one can visualize the alignment angle of the atomic p charge cloud in terms of a transition from a body fixed molecular picture (small internuclear distances R) to a space fixed picture (large R). These concepts are illustrated by experimental results for $e + Na^+$ and $Na + Na^+$ collisions. Further examples are the molecular processes $N_2 + Na^+$ and the atomic process $Xe + Ba^+$ at thermal energies.

500,446

PB86-124005

Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Molecular Spectroscopy Div.

NO Thermally Desorbed from a Saturation Coverage on Pt(111): Internal State Distributions.

Final rept.,
D. S. King, D. A. Mantell, and R. R. Cavanagh. 1985, 3p
Contract DE-A105-84ER13150
Sponsored by Department of Energy, Washington, DC.
Pub. in Jnl. of Chemical Physics 82, n2 p1046-1048, 15 Jan 85.

Keywords: *Nitrogen oxides(NO), *Desorption, *Surface chemistry, Platinum, Thermochemistry, Reprints.

No abstract available.

500,447

PB86-124013

Not available NTIS

National Bureau of Standards (NML), Gaithersburg, MD. Inorganic Analytical Research Div.

Elemental Rationing Technique for Assessing Concentration Data from a Complex Water System.

Final rept.,
H. M. Kingston, and R. R. Greenberg. 1984, 9p
Pub. in Environment International 10, p153-161 1984.

Keywords: *Water analysis, Concentration(Composition), Sites, Sampling, Chemical analysis, Sediments, Particles, Assessments, Comparison, Reprints, *Water pollution sampling, *Water pollution detection.

Water samples have been collected at the surface and bottom layers at 51 locations throughout Chesapeake Bay. The suspended particulate and dissolved fractions of these samples have been analyzed for Cd, Ce, Co, Cu, Fe, Mn, Mo, Ni, Pb, Sc, Sn, Th, U, and Zn using neutron activation analysis and atomic absorption spectrometry. Special chemical procedures were used to preconcentrate the elements of interest in the dissolved samples and separate them from the salt water matrix. The elemental concentrations observed in the dissolved samples were evaluated by direct comparison to those found in coastal seawater; however, the elemental concentrations in the particulate samples (mass per volume of water) were strongly influenced by the total amount of particulate material suspended in the water at time of collection. A double normalization procedure was used to calculate crustal enrichment factors for each sample, and these enrichment factors provided both a means to observe sample-to-sample variations, and also allowed a crude comparison with the natural levels occurring in the earth's crust.

500,448

PB86-124021

Not available NTIS
National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.

Fracture Strength and the Weibull Distribution of Beta-Sialon.

Final rept.,
K. Kobayashi, S. Umehayashi, K. Kishi, N. J. Tighe, and R. J. Fields. 1981, 6p
Pub. in Yogyo Kyokaiishi 89, n10 p550-555 1981.

Keywords: *Chemical bonds, *Fracture strength, Weibull density functions, High temperature tests, X ray analysis, Reprints, *Sialon, Aluminum silicon oxynitride.

4 point bend strength and the Weibull distribution were measured for hot-pressed beta-sialon (Si₅Al₁₀N₇) at room temperature, 1200C and 1400C in air. The hot-pressed beta-sialon was fabricated from SiO₂, Al and Si powders in N₂. The hot-pressed sample consisted of single beta-sialon as a crystalline phase by X-ray analysis, but glassy grain boundary phase was detected by SEM observation.

500,449

PB86-124047

Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Molecular Spectroscopy Div.

Doppler-Limited Study of the Infrared Spectrum of Allene from 2965 to 3114 /cm.

Final rept.,
A. G. Maki, A. S. Pine, and M. Dang-Nhu. 1985, 23p
Pub. in Jnl. of Molecular Spectroscopy 112, p459-481 1985.

Keywords: *Infrared spectroscopy, *Doppler effect, *Allene, Molecular structure, Molecular energy levels, Reprints, *Laser spectroscopy.

A difference-frequency laser spectrometer has been used to measure the infrared absorption spectrum of the ν (sub 5) and ν (sub 8) bands of allene (C₃H₄).

500,450

PB86-124112

Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Molecular Spectroscopy Div.

Torsional-Wagging Tunneling Problem and the Torsional-Wagging-Rotational Problem in Hydrazine.

Final rept.,
N. Ohashi, and J. Hougen. 1985, 17p
Pub. in Jnl. of Molecular Spectroscopy 112, p384-400 1985.

Keywords: *Hydrazine, *Molecular rotation, *Molecular vibration, Molecular energy levels, Reprints.

Results derived previously for the rotational levels of the eight-framework and three-large-amplitude vibra-

tional problem in N₂H₄, using a tunneling formalism based on a treatment of the vibration-rotation problem as a whole, are rederived here in a much simpler fashion, using a tunneling formalism based on a separate treatment of the vibrational and rotational problems. The present formalism is thus much more akin to the usual vibration-rotation formalism, and the origins of the various contributions to the vibration-rotation energy levels can be understood relatively easily. It is convenient here, as earlier, to make extensive use of permutation-inversion and extended-group (double-group) ideas, but it is necessary in the present treatment to consider tunneling between 16 minima in molecular coordinate space, i.e., between a number of minima which is twice the number of nonsuperimposable molecular frameworks that can actually be constructed for N₂H₄. (Copyright (c) Academic Press, Inc. 1985.)

500,451

PB86-124120

Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Inorganic Materials Div.

Characterization of Bioactive Organotin Polymers: Fractionation and Determination of MW by SEC (Size Exclusion Chromatography)-GFAA.

Final rept.,
E. J. Parks, and F. E. Brinckman. 1981, 20p
See also AD-A089164.
Pub. in Proceedings of International Symposium on Controlled Release Pestic. Pharm. (7th), p219-238 1981.

Keywords: *Copolymers, *Polymerization, *Molecular weight, *Distillation, *Tin organic compounds, Chromatographic analysis, Polymethyl methacrylate, Concentration(Composition), Ultraviolet spectroscopy, Sampling, *Free radicals, *Size exclusion chromatography, *Graphite furnace spectroscopy, Methyl methacrylates, Biological processes, Methacrylic acid/(methacryloyloxy).

Organotin polymers (OMP's) prepared by the free radical copolymerization of methyl methacrylate (MMA) with tributyltin methacrylate (TBTM) and/or tripropyltin methacrylate (TPTM) were subjected to size exclusion chromatography (SEC) in tetrahydrofuran as solvent and mobile phase, with continuous eluant monitoring by ultraviolet (UV) and tin-specific graphite furnace (GFAA) spectrophotometry.

500,452

PB86-124757

Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Organic Analytical Research Div.

Photodissociation of the Molecular Ion of n-Butylbenzene: Effect of Photon Energy.

Final rept.,
M. J. Welch, D. J. Pereles, and E. White. 1985, 2p
Pub. in Organic Mass Spectrometry 20, n6 p425-426 1985.

Keywords: *Photochemical reactions, *Dissociation, Ions, Mass spectroscopy, Photons, Reprints, *Benzene/butyl, *Laser spectroscopy.

The authors investigated the photon-induced dissociation of the n-butylbenzene molecular ion. An argon ion laser was used to irradiate the first field-free region of a Mattauch-Herzog geometry mass spectrometer. Only source temperatures had a significant effect, but temperature differences were not enough to account for the differences between our results and those previously reported, which were obtained in the second field-free region of a reverse geometry instrument. The reasons for the discrepancies are not understood.

500,453

PB86-124773

Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Gas and Particulate Science Div.

Quality Assurance Measures for Environmental Data.

Final rept.,
J. K. Taylor. 1980, 5p
Pub. in Proceedings of International Experts Discussion on Lead Occurrence, Fate, and Pollution in the Marine Environment, Rovinj, Yugoslavia, October 18-22, 1977, p1-5 1980.

Keywords: *Quality assurance, *Environmental surveys, *Chemical analysis, *Quality control, Sampling, *Toxic substances.

An understanding of the occurrence, fate, effects and pollution potential of a suspected toxic substance re-

quires a wide variety of analytical data. Stringent requirements are placed upon its reliability if data are to be intercompared and correlated. The quality assurance measures with respect to sampling and measurement are discussed.

500,454
PB86-124922 Not available NTIS
National Bureau of Standards (NEL), Boulder, CO.
Chemical Engineering Science Div.

Thermal Conductivity of Hydrogen for Temperatures between 78 and 310 K with Pressures to 70 MPa.

Final rept.,
H. M. Roder. 1984, 28p
Sponsored by National Aeronautics and Space Administration, Washington, DC.
Pub. in International Jnl. of Thermophysics 5, n4 p323-350 Dec 84.

Keywords: *Hydrogen, *Thermal conductivity, *Laboratory equipment, Temperatures, Pressures, Experimental design, Isotherms, Density(Mass/volume), Reprints.

The paper presents new experimental measurements of the thermal conductivity of hydrogen. The ortho-para compositions covered are normal, near normal, para, and para-rich. The measurements were made with a transient hot wire apparatus. The temperatures covered the range from 78 to 310 K with pressures to 70 MPa and densities from 0 to a maximum of 40 mol/L. For compositions normal and near normal, the isotherms cover the entire range of pressure, and the temperatures are 78, 100, 125, 150, 175, 200, 225, 250, 275, 294, 300, and 310 K. The para measurements include eight isotherms at temperatures from 100 to 275 K with intervals of 25 K, pressures to 12 MPa, and densities from 0 to 12 mol/L. Three additional isotherms at 150, 250, and 275 K cover para-rich compositions with para percentages varying from 85 to 72%. For these three isotherms the pressures reach 70 MPa and the density a maximum of 30 mol/L. The data for all compositions are represented by a single thermal conductivity surface. The data are compared with the experimental measurements of others through the new correlation. The precision (2 sigma) of the hydrogen measurements is between 0.5 and 0.8% for wire temperature transients of 4 to 5 K, while the accuracy is estimated to be 1.5%.

500,455
PB86-125150 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Thermophysics Div.

Scaled Fundamental Equation for the Thermodynamic Properties of Steam Near the Critical Point.

Final rept.,
J. V. Sengers, J. M. H. Levelt Sengers, and B. Kamgar-Parsi. 1985, 15p
Sponsored by National Science Foundation, Washington, DC.
Pub. in Strojnický Casopis 36, n3 p277-291 1985.

Keywords: *Critical point, *Thermodynamic properties, *Steam, Surface chemistry, Scaling, Comparison, Reprints, Numerical solution.

The modern theory of critical phenomena asserts that the thermodynamic surface of fluids near the critical point is characterized by scaling laws with universal critical exponents and universal scaling functions. The paper reviews results obtained with a scaled fundamental equation for steam in the critical region. A comparison with a new formulation adopted by IAPS for the thermodynamic properties of water substance is also included.

500,456
PB86-128113 Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Chemical Engineering Science Div.

Density Expansion (DEX) Mixing Rules: Thermodynamic Modeling of Supercritical Extraction.

Final rept.,
G. A. Mansoori, and J. F. Ely. 1985, 8p
Sponsored by National Science Foundation, Washington, DC.
Pub. in Jnl. of Chemical Physics 82, n1 p406-413, 1 Jan 85.

Keywords: *Mathematical models, *Thermodynamics, *Density(Mass/volume), Solubility, Mixtures, Reprints, *Supercritical gas extraction.

Conformal solution theory and the density expansion expression of the radial distribution function of fluids

are used to derive a set of mixing rules. The new mixing rules are composition, density, and temperature dependent. To test the new mixing rules they are used for thermodynamic modeling of supercritical extraction. Comparison of the result of calculation by the mixing rules with the van der Waals mixing rules indicates a profound improvement over the latter in prediction of properties of mixtures consisting of species with large molecular size and shape differences.

500,457
PB86-128121 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Inorganic Analytical Research Div.

Use of Isotope Dilution Mass Spectrometry for the Certification of Standard Reference Materials.

Final rept.,
L. J. Moore, H. M. Kingston, T. J. Murphy, and P. J. Paulsen. 1984, 5p
Pub. in Environment International 10, p169-173 1984.

Keywords: *Environmental surveys, *Trace elements, *Chemical analysis, Lead(Metal), Water analysis, Fly ash, Mercury(Metal), Uranium, Air pollution, Gas analysis, Concentration(Composition), Reprints, *Isotope dilution mass spectrometry, *Standard reference materials, *Natural emissions, SRM 1643, SRM 1633a, SRM 1577a, SRM 1642.

Isotope dilution mass spectrometry (IDMS) has been used extensively at the U.S. National Bureau of Standards as an accurate method to determine trace element concentrations in natural materials. Thermal ionization mass spectrometry is a single element technique capable of high accuracy and precision, and has been used for 'definitive' measurements of trace elements in sera with 95% confidence limits less than 0.25%. Spark source mass spectrometry is a complementary multielement, high-sensitivity technique that has been used to determine up to 20 elements in a sample, with typical accuracies of 2%-5%. Together with appropriate chemical separations, such as anion and cation exchange, chelate resins, electrodeposition, and chemical extraction, IDMS has been applied to elemental concentration measurements ranging over eight orders of magnitude, from decigrams/gram to picograms/gram. Many of these applications have been used for the certification of a broad spectrum of biological and environmental Standard Reference Materials, including lead in Trace Elements in Water (SRM 1643), 15 elements in Coal Fly Ash (SRM 1633a), uranium in Bovine Liver (SRM 1577a), and mercury in water (SRM 1642).

500,458
PB86-128139 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Organic Analytical Research Div.

Optically Transparent Thin-Layer Electrode for Organic Solvents.

Final rept.,
E. P. Muth, J. E. Fuller, L. M. Doane, and E. A. Blubaugh. 1982, 2p
Pub. in Analytical Chemistry 54, p604-605 1982.

Keywords: *Organic solvents, *Electrodes, Thin layer chromatography, Optical materials, Reprints.

An optically transparent thin layer electrode for use in nonaqueous solvents is described.

500,459
PB86-128147 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Building Materials Div.

Degradation of Poly(Vinyl Fluoride) and Poly(Vinylidene Fluoride).

Final rept.,
T. Nguyen. 1985, 49p
Sponsored by Department of Energy, Washington, DC.
Pub. in JMS-Rev. Macromol. Chem. Phys. C25, n2 p227-275 1985.

Keywords: *Degradation, *Polyvinyl fluoride, *Chemical analysis, *Construction materials, Comparison, Additives, Impurities, Copolymers, Reprints, *Vinylidene fluoride polymers.

Available literature on the degradation of vinyl fluoride and vinylidene fluoride homo- and copolymers has been reviewed. It is apparent from these data that the thermal and high-energy radiation degradation of these materials have been extensively investigated; however, other types of degradation have not been investigated in depth. The data reviewed reveal several problems for workers interested in these materials. (1)

Lack of information on the combined effects of UV and temperature, UV and moisture, or of the combined three factors. (2) Methods used for the detection and characterization of the degradation varied from mechanical tests to spectral analysis, and the results of these analyses can not be compared from one to another. (3) Inability to compare the results of the various studies, due to differences in materials, preparation methods, test conditions and sample sizes used for the analyses by various authors. The presence of additives and impurities, and recent advancements in processing and method of preparation of these materials compound the problem of interpreting and comparing various studies. Research is needed to address the three key problems cited above.

500,460
PB86-128162 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Building Materials Div.

Applications of Fourier Transform Infrared Spectroscopy in Surface and Interface Studies.

Final rept.,
T. Nguyen. 1985, 34p
Pub. in Progress in Organic Coatings 13, p1-34 1985.

Keywords: *Infrared spectroscopy, *Chemical analysis, *Surface chemistry, *Organic coatings, Reviews, Reprints, *Fourier transform spectroscopy.

The development of Fourier transform infrared (FTIR) spectrometers, which have superior sensitivity, more rapid sample measurement and more versatile spectral processings, has revised interest of infrared spectroscopy as an analytical method for surface and interface studies. The article will briefly review the background of FTIR and extensively review the current literature on the applications of FTIR spectroscopy for surface and interface studies. The literature surveyed in this review indicates the strength and suitability of FTIR, coupled with appropriate IR spectroscopic technique for surface and interface studies. The selection of a specific technique for a particular surface application depends upon factors such as sample nature and morphology and sensitivity required. Despite remarkable advancement of FTIR instrumentation, the applications of this technique in surface and interface studies are still in the infancy stage. With much interest in obtaining molecular level information in a wide range of materials applications, FTIR spectroscopy is expected to be increasingly utilized for providing qualitative and quantitative molecular information on the surface and interface of materials.

500,461
PB86-128204 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Inorganic Analytical Research Div.

Application of Atomic Absorption and Plasma Emission Spectrometry for Environmental Analysis.

Final rept.,
T. C. Rains, R. L. Watters, and M. S. Epstein. 1984, 6p
Pub. in Environment International 10, p163-168 1984.

Keywords: *Environmental surveys, *Chemical analysis, Trace elements, Leaching, Urban areas, Wear metals, Lubricating oils, Reprints, *Standard reference materials, Inductively couple plasma emission spectroscopy, Flame atomic absorption spectrometry, Solid wastes, Air pollution detection, SRM 1648, SRM 1084, SRM 1085, Electrothermal atomization.

The application of flame atomic absorption (FAAS), electrothermal atomic absorption (ETAAS), inductively coupled plasma emission (ICP), and direct-current plasma emission spectrometry (DCP) for the determination of major, minor, and trace elements in Urban Particulates (SRM 1648), Wear Metals in Oil (SRM 1084 and 1085), and Simulated Solid-Waste Leachates is described. Interferences were encountered in the determination of the trace elements in SRM 1648 by ETAAS; however, these interferences were alleviated using a 1% solution of ammonium dibasic phosphate as a matrix modifier. The concentration of elements in SRM 1084 and 1085 and the simulated solid-waste leachates were significantly above the detection limits by FAAS or ICP and no analytical difficulty was encountered.

500,462
PB86-128246 Not available NTIS

Field 7—CHEMISTRY

Group 7D—Physical Chemistry

National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.

Detailed Look at Aspects of Optical Pumping in Sodium.

Final rept.,

J. J. McClelland, and M. H. Kelley. 1985, 7p
Sponsored by Department of Energy, Washington, DC.
Office of Basic Energy Sciences.

Pub. in Physical Review A: General Physics 31, n6
p3704-3710 Jun 85.

Keywords: *Optical pumping, *Sodium, Ground state, Electron spin, Polarization(Spin alignment), Reprints, Bloch equations, Laser radiation.

Calculations and measurements are presented of the increase in $(F \text{ bar})=1$ ground-state population as a function of incident laser intensity in optically pumped sodium. The calculations involve numerical integration of a multilevel version of the optical Bloch equations. Agreement between experiment and theory is good when proper account is taken of the residual Doppler width in the atomic beam, which causes a larger increase in the $(F \text{ bar})=1$ population. The $(F \text{ bar})=1$ population increases by 3.5% at 35 mW/sq cm, the highest laser intensity investigated.

500,463

PB86-128741

PC A04/MF A01

National Bureau of Standards (NML), Gaithersburg, MD. Center for Analytical Chemistry.

International Review of Environmental Specimen Banking.

Final rept.,

S. A. Wise, and R. L. Zeisler. Oct 85, 65p NBS/SP-706

Also available from Supt. of Docs as SN003-003-02693-0. Library of Congress catalog card no. 85-600601. Sponsored by Environmental Protection Agency, Washington, DC.

Keywords: *Environmental surveys, *International relations, *Meetings, Reviews, Samples, Trends, Inorganic analysis, Organic analysis, Chemical analysis.

In September 1983, the '8th U.S. - German Seminar of State and Planning on Environmental Specimen Banking' and the 'International Review of Environmental Specimen Banking' were held at the National Bureau of Standards. At these meetings the current status of Environmental Specimen Banking Program in the U.S., Federal Republic of Germany (FRG), and other countries was presented and discussed. The publication contains a brief summary of these meetings and separate contributions describing the specimen banking activities in Canada, FRG, Japan, Sweden and the U.S.

500,464

PB86-128832

Not available NTIS

National Bureau of Standards (NEL), Gaithersburg, MD. Fire Measurement and Research Div.

Calculations of the Dimerization of Aromatic Hydrocarbons: Implications for Soot Formation.

Final rept.,

J. H. Miller, K. C. Smyth, and W. G. Mallard. 1984, 9p

Pub. in Proceedings of International Symposium on Combustion/The Combustion Institute (20th), Ann Arbor, MI., August 1984, p1139-1147 1985.

Keywords: *Aromatic polycyclic hydrocarbons, *Soot, *Air pollution, Combustion, Flames, Van der Waals forces, Equations of state, Nucleation, Concentration(Composition), Monomers, Hydrocarbons, Dimers, Chemical reaction mechanisms.

Polynuclear aromatic hydrocarbons (PAH) are found in all sooting hydrocarbon flames. These species are ideally suited to be chemical precursors and building blocks in soot formation, yet their possible role has not been elucidated. From a knowledge of the magnitude of the van der Waals interaction between pairs of PAH the equilibrium constants for dimer formation have been calculated. These values have been used with experimentally measured PAH concentrations to compute dimer concentrations, which were then compared to soot nuclei number densities to determine whether or not the dimers are numerous enough to serve as nucleation sites. The dimers of benzene coronene (7 rings), and circumcoronene (19 rings), as well as mixed dimer pairs, have been examined. Despite choosing monomer concentrations and theoretical approaches which favor dimer formation, the dimerization of PAH does not yield a sufficient number of nucleation sites to account for soot formation in a homogeneous nucleation mechanism. If PAH do participate in the early

stages of soot formation, irreversible chemical steps must be important.

500,465

PB86-128840

Not available NTIS

National Bureau of Standards, Gaithersburg, MD. Polymers Div.

Dielectric Properties of Polymers at Microwave Frequencies: A Review.

Final rept.,

A. J. Bur. 1985, 15p

Sponsored by Construction Engineering Research Lab. (Army), Champaign, IL.

Pub. in Polymer 26, p963-977 Jul 85.

Keywords: *Polymers, *Dielectric properties, *Microwave frequencies, Reviews, Reprints.

A review of the dielectric loss spectra of polymers at microwave frequencies has been carried out. While the main focus of attention is the frequency range from 100 MHz to 100 GHz, loss spectra outside this region are also reviewed because variations in temperature can cause a shift of dielectric loss into or out of the microwave range. A large volume of data for low loss polymers (polyethylene, polypropylene and poly(tetrafluoroethylene)), which are used in the communications industry, was available for review. Also, the microwave dielectric properties of engineering thermoplastics such as poly(phenylene oxide), polycarbonate and polysulphane have been reviewed. The origins of microwave dielectric loss in polymers are categorized as: (a) dipolar absorption dispersions in both crystalline and amorphous polymers; (b) dipolar losses due to impurities, additives or fillers in a polymer material; (c) microwave absorption in conducting polymers (polyacetylene and poly(sulphur nitride)) for which the current carriers are electrons; and (d) photon-phonon absorption spectra corresponding to the density of states in amorphous regions of a polymer material.

500,466

PB86-128931

Not available NTIS

National Bureau of Standards (NML), Gaithersburg, MD. Office of Standard Reference Materials.

Role of NBS (National Bureau of Standards) Standard Reference Materials in Quality Assurance of Environmental Measurements.

Final rept.,

R. Alvarez. 1985, 14p

Pub. in Quality Assurance for Environmental Measurements, ASTM STP 867, p346-359 1985.

Keywords: *Quality assurance, *Environmental surveys, *Chemical analysis, Sampling, Gas analysis, Water analysis, Trace elements, Laboratory equipment, Fuels, Bioassay, Sediments, Halocarbons, Aromatic polycyclic hydrocarbons, Sampling, Reprints, *Standard reference materials, Water pollution detection, Air pollution detection.

Analyses of environmental samples of known homogeneity by different laboratories often disagree seriously. Discrepant data may result from poor methodology, improper instrument calibration, faulty experimental techniques, or from a combination of these factors. One approach towards obtaining accurate data is through the use of Standard Reference Materials (SRMs) issued by the National Bureau of Standards under federal statutes. SRMs are homogeneous, stable materials with certified chemical or physical properties and are used in calibrating instruments, validating laboratory data, developing methods of known accuracy, and referring data from different laboratories to a common base. Of the approximately 900 SRMs listed in the current SRM catalog, over 90 have been developed for use in improving the accuracy of environmental analyses. Environmental matrix SRMs certified for priority pollutants include gases, atmospheric dust, water, sediments, biological materials, and fuels. In addition, calibrator solutions of organic priority pollutants, such as halocarbons, and polycyclic aromatic hydrocarbons, are available for determining instrumental response factors, and adding accurate amounts of these compounds to samples.

500,467

PB86-128980

Not available NTIS

National Bureau of Standards (NML), Boulder, CO. Time and Frequency Div.

Laser-Cooled Stored Ion Experiments Using Penning Traps.

Final rept.,

J. J. Bollinger, D. J. Wineland, and W. M. Itano. 1983, 4p

Sponsored by Air Force Office of Scientific Research, Bolling AFB, DC., and Office of Naval Research, Arlington, VA.

Pub. in Proceedings of International Conference on Lasers '83, San Francisco, CA., December 12-16, 1983, p727-730.

Keywords: Frequency standards, Mass spectroscopy, *Ion storage, Ion traps, Penning traps, Laser cooling, Beryllium 9, Plasma.

Small clouds of 9Be^+ ions are stored in a Penning trap and cooled with a laser to temperatures below 200 mK. The ions are detected by their fluorescence induced by the cooling laser. Experiments on high resolution spectroscopy and frequency standards, mass spectroscopy, and one-component plasmas are discussed.

500,468

PB86-129509

Not available NTIS

National Bureau of Standards (NEL), Gaithersburg, MD. Chemical Process Metrology Div.

Interaction of Water Vapor with Tin Oxide.

Final rept.,

D. F. Cox, S. Semancik, and P. D. Szuromi. 1985, 4p

Pub. in Proceedings of International Conference on Solid-State Sensors and Actuators-Transducers '85, Philadelphia, PA., June 11-14, 1985, p385-388.

Keywords: *Tin oxides, *Water vapor, Interactions, Adsorption, Surfaces, Valence bands, Auger electron spectroscopy, Photoelectron spectroscopy.

The interactions of low coverages of water vapor with tin oxide have been studied at temperatures below 200K. Auger electron spectroscopy (AES) and ultraviolet photoelectron spectroscopy (UPS) were used to characterize the clean tin oxide surface, and UPS was used to monitor the water adsorption process. Changes in the valence band UPS spectra induced by the molecular water overlayers are discussed.

500,469

PB86-129640

Not available NTIS

National Bureau of Standards, Gaithersburg, MD. Polymers Div.

Neutron Scattering from Polymers.

Final rept.,

R. S. Stein, and C. C. Han. 1985, 8p

Pub. in Physics Today, p1-8 Jan 85.

Keywords: *Neutron scattering, *Polymers, Solutions, Melts, Gels, Crystals, Deuterium compounds, Reprints.

The great difference in scattering power between a deuterated polymer and its hydrogenous counterpart allows one to determine the shapes and movements of polymers in solutions, melts, gels, and crystals.

500,470

PB86-129657

Not available NTIS

National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.

Linear-Versus-Nonlinear Regime in Macroscopic Quantum Fluctuations of Stokes Pulses.

Final rept.,

M. Trippenbach, and K. Rzazewski. 1985, 4p

Pub. in Physical Review A: General Physics 31, n3
p1932-1935 Mar 85.

Keywords: *Quantum, *Mathematical models, *Stokes law(Fluid mechanics), *Raman scattering, Dynamics, Reprints.

An explicitly soluble model of macroscopic quantum fluctuations of Stokes pulses is presented. The model deals with a small sample placed in a cavity and covers both linear and nonlinear regimes. The energy distribution of pulses narrows in the nonlinear regime, which is in agreement with the recent experiments.

500,471

PB86-130135

Not available NTIS

National Bureau of Standards (NML), Boulder, CO. Time and Frequency Div.

Heterodyne Frequency Measurements on N₂O at 5.3 and 9.0 Micrometers.

Final rept.,
J. S. Wells, D. A. Jennings, A. Hinz, J. S. Murray, and A. G. Maki. 1985, 5p
Sponsored by National Aeronautics and Space Administration, Washington, DC.
Pub. in Jnl. of the Optical Society of America B2, n5 p857-861 May 85.

Keywords: *Nitrogen oxide(N₂O), *Infrared spectroscopy, Calibrating, Molecular vibration, Absorption, Standards, Performance evaluation, Reprints, *Laser spectroscopy, Heterodynereactions.

Heterodyne frequency measurements on the 01(sup 1)1-00(sup 0)0 band of N₂O have been made with the use of a tunable-diode laser, a CO laser transfer oscillator, and a CO₂ laser frequency synthesizer. A beat frequency was measured between a CO laser and a tunable-diode laser whose frequency was locked to the peak of N₂O absorption features. The frequency of the CO laser was simultaneously determined by measuring the beat frequency with respect to a reference synthesized from two CO₂ lasers. New rovibrational constants are given for the 01(sup 1)1 state of N₂O, which are in excellent agreement with previous results, although the band center is 4 MHz higher than in the previous measurements. A table of the line frequencies and their absolute uncertainties is given for the N₂O absorption lines in the wave-number region from 1830 to 1920/cm. Some additional frequency measurements near the lower-frequency end of the 02(sup 0)0-00(sup 0)0 band have also been made with respect to a (12 sup)C(18 sup)O₂ laser.

500,472

PB86-130168

Not available NTIS
National Bureau of Standards (NML), Boulder, CO.
Time and Frequency Div.

High-Resolution Spectroscopy of Stored Ions.

Final rept.,
D. J. Wineland, W. M. Itano, and R. S. Van Dyck. 1983, 52p

Sponsored by Air Force Office of Scientific Research, Bolling AFB, DC., Office of Naval Research, Arlington, VA., and National Science Foundation, Washington, DC.

Pub. in Advances in Atomic and Molecular Physics 19, p135-186 1983.

Keywords: Mass spectroscopy, Magnetic moments, Electrons, Positions, *Ion storage, Ion traps, Ion spectroscopy, High resolution.

The paper gives a review of high resolution spectroscopy experiments that have employed the stored ion technique. The main elements of the paper are Sections on (1) storage techniques, (2) lepton spectroscopy, (3) mass spectroscopy (4) atomic and molecular spectroscopy (5) negative ion spectroscopy (6) radiative lifetime measurements.

500,473

PB86-130937

PC A13/MF A01
National Bureau of Standards (NML), Gaithersburg, MD. Office of Standard Reference Data.

Chemical Thermodynamics in Steam Power Cycles Data Requirements.

O. Jonas, and H. J. White. Jul 85, 291p NBSIR-85/3205

Proceedings of a workshop held at National Bureau of Standards, Gaithersburg, Maryland, February 8-9, 1983. Sponsored by American Society of Mechanical Engineers, New York, and Electric Power Research Inst., Palo Alto, CA.

Keywords: *Thermodynamics, *Meetings, *Steam electric power generation, *Corrosion, *Impurities, *Industrial waste treatment, Tables(Data), Materials tests, Water pollution control, Experimental design, Nuclear power plants, Boilers, Marine engines, *Reference materials, *Chemical treatment.

The report represents the proceedings of a workshop on data needs for chemical thermodynamics in power cycles held at the National Bureau of Standards, February 8-9 1983. It contains a summary of the recommendations of working groups that met during the workshop as well as the texts or abstracts of most of the papers presented at the workshop.

500,474

PB86-132214

Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Inorganic Materials Div.

Electrolytic Coloration and Electrical Breakdown in MgO Single-Crystals.

Final rept.,
M. M. Abraham, L. A. Boatner, W. H. Christie, F. A. Modine, and T. Negas. 1984, 16p
Sponsored by Oak Ridge National Lab., TN.
Pub. in Jnl. of Solid State Chemistry 51, n1 p1-16 1984.

Keywords: *Magnesium oxides, Electrical faults, Dielectric breakdown, Single crystals, Impurities, Reprints, *Breakdown(Electronic threshold), Doped materials.

A series of investigations of electrolytic coloration effects product in MgO single crystals containing iron-group impurities has been carried out. The purpose of these investigations was to determine the identity and production mechanism of localized coloration or dark streaks that are frequently observed following the electrical breakdown of MgO crystals at temperatures in the range of 1000 C.

500,475

PB86-132222

Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Semiconductor Devices and Circuits Div.

Alternative Approach to the Calculation of Four-Probe Resistances on Nonuniform Structures.

Final rept.,
J. Albers, and H. L. Berkowitz. 1985, 4p
Pub. in Jnl. of the Electrochemical Society: Solid-State Science and Technology 132, n10 p2453-2456 Oct 85.

Keywords: *Electrical resistivity, *Structural analysis, *Probes, Calibrating, Substitutes, Electrochemistry, Reprints, *Spreading resistance, Numerical solution.

An alternative approach to the calculation of the four-probe resistance of nonuniform resistivity structures is presented. This approach is based upon two simplifications in the form of the four-probe resistance integral. The first arises from the integral's being independent of the probe current density as well as the probe radius. The second simplification involves the rewriting of the integral as one involving only the kernel (without any Bessel functions) and with finite limits which depend only upon the probe spacing. The form of these limits is determined by analytic calculation of the four-probe resistance for the case of a semi-infinite slab. For the case of a uniform layer over an insulating or conducting boundary, the simplified integral leads to analytic expressions for the four-probe resistance which are compared with the more extensive technique and are also investigated as a function of the probe spacing. For nonuniform resistivity structures, the simplified integral can be easily evaluated by means of the Newton-Cotes numerical procedure. For general multilayer cases, the results obtained from the Newton-Cotes method are compared with those obtained from more extensive numerical techniques and are shown to be in excellent agreement. This allows for a vastly simplified implementation of the previously proposed spreading resistance calibration technique.

500,476

PB86-132230

Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Semiconductor Materials and Processes Div.

Investigation of the Relation between the Correction Factor and the Local Slope in Spreading Resistance.

Final rept.,
J. Albers. 1983, 1p
Pub. in Jnl. of the Electrochemical Society 130, n8 pC327 1983.

Keywords: *Correction, *Mathematical models, *Electrical resistivity, Electrochemistry, Reprints, *Spreading resistance, *Local slope, Laplace equation.

The local slope method for the calculation of the spreading resistance correction factor has been proposed by Dickey. The method is based on two asymptotic models for the conduction process involved in the spreading resistance measurement for the cases of (1) a conducting layer over an insulating substrate, and (2) a high resistivity layer over a low resistivity or conducting substrate. The two extreme cases are bridged by means of an assumed single-valued relation between the correction factor and the local slope of the spreading resistance data. The paper examines the two asymptotic models and the assumed single-valued relation in terms of the multilayer Laplace equation description of spreading resistance. It is shown that the asymptotic models adequately describe the behavior of the correction factor for a thin uniform layer over

insulating or conducting boundaries. In addition, the single-valued relation between the correction factor and the local slope which is assumed by the local slope method is shown not to be an adequate representation of the multiple-valued relation between these two quantities found from the Laplace equation description. A comparison of the two correction factor vs. local slope relations provides the basis for the understanding of the results of these schemes when model spreading resistance data are used. Nonetheless, the local slope results qualitatively follow the multilayer results thus making the technique a usable one for the calculation of approximate correction factors.

500,477

PB86-132248

Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.

Coherence Study of 2p(sigma)-2p(pi) Rotational Coupling: Li(2 doublet P) and He(2 singlet P) Orientation and Alignment in 1-25 keV Li(+1)-He Collisions.

Final rept.,
N. Andersen, T. Andersen, H. Neitzke, and E. H. Pedersen. 1985, 23p
Pub. in Jnl. of Physics B: Atomic and Molecular Physics 18, n11 p2247-2269 1985.

Keywords: *Molecular energy levels, *Lithium, *Helium, Molecular rotation, Reprints, *Ion molecule collisions, Lithium ions.

The authors have studied the alignment and orientation of the electron cloud of the Li(2 doublet P) and He(2 singlet P) states excited by 2p(sigma)2p(pi) rotational coupling for impact parameters between 0.2 and 1.1 au in 1-25 keV Li(+1)-He collisions by coherence and correlation analysis techniques. It is found that for collision energies below 5 keV the shape of the excited electron cloud is very nearly that of a p orbital, aligned perpendicular to the asymptotic internuclear axis, independent of impact parameter and of whether the electron stays on the He core or is transferred to the Li centre during the collision. These findings agree with the predictions based on an analysis of the simple diabatic MO diagram for the Li-He system. At energies above 5 keV, the shape changes significantly. Also, the alignment angle deviates from the perpendicular direction, being larger than 90 deg for Li and smaller for He. The angular momentum perpendicular to the collision plane shows a pronounced variation with collision energy but is only weakly dependent on impact parameter. Possible origins for this behavior are discussed.

500,478

PB86-132255

Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.

Multiply Excited Three-Electron Systems Studied by Optical Emission Spectroscopy.

Final rept.,
T. Andersen, and S. Mannervik. 1985, 14p
Pub. in Comments on Atomic and Molecular Physics 16, n4 p185-198 1985.

Keywords: *Emission spectroscopy, *Molecular energy levels, *Lithium, *Boron, *Beryllium, Excitation, Reprints.

Recent developments in the study of radiative multiply excited states in three-electron systems are reviewed. The progress concerns experimental and theoretical studies of the term schemes for quartet states in Li I, Be II, and B III, the first term schemes for doublet states in Li I and Be II, absolute term values for Li I, the existence of two bound states in Li(-1), and the first accurate autoionization widths for autoionizing resonances in Li I and Be II. This comment concentrates on the low Z numbers for which strong effects of electron correlation and configuration interactions are important.

500,479

PB86-132263

Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymer Science and Standards Div.

Native Cellulose - A Composite of 2 Distinct Crystalline Forms.

Final rept.,
R. H. Atalla, and D. L. VanderHart. 1984, 3p
Pub. in Science 223, n4633 p283-285 1984.

Field 7--CHEMISTRY

Group 7D--Physical Chemistry

Keywords: *Cellulose, *Carbon 13, *Crystal structure, *Nuclear magnetic resonance, *Isotopic labeling, Plants(Botany), Bacteria, Algae, Reprints.

Multiplicities in the resonances of chemically equivalent carbons, which appear in the solid state (sup 13)C NMR spectra of native celluloses have been examined at high resolution. The patterns of variation are consistent with existence of two distinct crystalline forms in native celluloses. One of the two forms is dominant in bacterial and algal celluloses, while the other form is dominant in celluloses from high plants.

500,480

PB86-132271

Not available NTIS

National Bureau of Standards (NML), Gaithersburg, MD. Center for Chemical Physics.

Radiation-Induced Ionization and Excitation in Liquid p-Dioxane.

Final rept.,

P. Ausloos, C. Lutz, F. Schwarz, and S. G. Lias.

1984, 8p

Pub. in Radiation Physics and Chemistry 23, n1-2 p97-104 1984.

Keywords: *Ionization, *Dioxanes, *Ultraviolet spectroscopy, Liquid phases, mixtures, Excitation, Molecular energy levels, Water, Reprints, *Dioxane, *Fluorescence induced ionization.

The fluorescence of neat liquid p-dioxane and p-dioxane-water mixtures has been studied as a function of wavelength in the range 200-110 micrometers, and in the system under beta irradiation. It is seen that the quantum yield of fluorescence declines from the absorption threshold to the ionization onset (about 160-170 micrometers), because of the increasing importance of the competing decomposition processes. Above the ionization onset, there is a slight increase in the quantum yield of fluorescence as a result of the occurrence of 'recombination fluorescence'. However, it is estimated that in the region, neutralization does not always lead to a vibrationally equilibrated excited state. This explains in part why the G-value of thermally equilibrated s(sub 1) states is considerably lower than G(ion)(about 5), under conditions that fluorescence originates mainly from charge recombination. Auxiliary experiments carried out in the gas phase, in an ion cyclotron resonance spectrometer, elucidated the reaction of p-C4H8O2 ions with p-dioxane molecules.

500,481

PB86-132487

Not available NTIS

National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.

Surface Chemistry of Water on Clean and Oxygen-Covered Copper (110).

Final rept.,

K. Bange, D. E. Grider, J. K. Sass, and T. E. Madey.

1984, 27p

Pub. in Surface Science 137, n1 p38-64 1984.

Keywords: *Surface chemistry, *Water, Copper, Adsorption, Desorption, Chemical reactions, Reprints.

Adsorption of water at 110 K on clean and oxygen-covered Cu(110) has been studied using UPS, TDS, delta phi and LEED measurements. A model of the arrangement of oxygen atoms and water molecules is presented, based upon the LEED observations for these layers and an estimate of the relative oxygen and water coverages. The intensity variation of a thermal desorption peak at 290 K, attributed to adsorbed OH-species, with oxygen coverage is in accordance with this model. For low oxygen coverages, the TDS and delta phi results indicate that small oxygen-water clusters with an enhanced ratio of water molecules per adsorbed oxygen atom are present.

500,482

PB86-132495

Not available NTIS

National Bureau of Standards (NML), Gaithersburg, MD. Semiconductor Materials and Processes Div.

Precise Evaluation of Oxygen Measurements on Cz-Silicon Wafers. Comments.

Final rept.,

A. Baghdadi. 1985, 1p

Pub. in Jnl. of the Electrochemical Society 132, n2 p510 1985.

Keywords: *Oxygen, *Chemical analysis, *Wafers, Infrared spectroscopy, Absorption, Performance evaluation, Silicon, Reprints.

This is a discussion of a paper by Graff, entitled 'Precise Evaluation of Oxygen Measurements on Cz-Silicon Wafers' which was published in the Journal of the Electrochemical Society, Vol. 130, No. 6, p. 1378. The equations used by Graff in his paper do not adequately represent the physical situation. This discussion points out the inconsistencies in Graff's approach to the problem.

con Wafers' which was published in the Journal of the Electrochemical Society, Vol. 130, No. 6, p. 1378. The equations used by Graff in his paper do not adequately represent the physical situation. This discussion points out the inconsistencies in Graff's approach to the problem.

500,483

PB86-132503

Not available NTIS

National Bureau of Standards (NML), Gaithersburg, MD. Inorganic Analytical Research Div.

Copper Standard Reference Materials (Benchmark Series).

Final rept.,

I. L. Barnes, T. E. Gills, and W. P. Reed. 1984, 10p

Pub. in Sampling and Analysis of Copper Cathodes, ASTM (American Society for Testing and Materials) STP 831, p145-154 1984.

Keywords: *Copper, *Standards, Chemical analysis, Metals, Reprints, *Standard reference materials.

The Standard Reference Materials Program has experienced increasing demands for new kinds and types of standard materials. In order that the largest number of users be served by these materials and the available resources be used to best advantage, careful planning is required. The planning process helps to ensure that, among other factors, the fewest number of different materials will be produced, a widerange of needs will be met, and production and certification can be accomplished at a level consistent with the intended uses. One output of this process has been the concept of 'Benchmark Series' SRMs. These are usually a set of similar materials with varying amounts of a number of elements covering a wide range of concentrations. Largely through the auspices of ASTM Committee E-2 on Emission Spectroscopy, more than 70 persons from NBS, ASTM, and from throughout the copper industry contributed to the planning of a series of Copper Benchmark Standard Reference Materials. As a result, 12 different materials issued as chips, rods, and cast solids and representing as many as 25 different SRMs have been prepared and certified for as many as 29 elements. The production and certification process and the certified values for this important series are described and the certified values are given.

500,484

PB86-132511

Not available NTIS

National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.

Interaction of Ammonia with Adsorbed Oxygen and Sodium on Ruthenium(001): Evidence for Both Local and Long-Range Interactions.

Final rept.,

C. Benndorf, and T. E. Madey. 1983, 6p

Pub. in Chemical Physics Letters 101, n1 p59-64 1983.

Keywords: *Ammonia, *Chemisorption, Ruthenium, Adsorption, Chemical bonds, Molecular structure, Atoms, Reprints, *Sodium atoms, *Atom molecule interactions, *Oxygen atoms.

The bonding geometry of adsorbed molecular NH3 on Ru(001) is changed in different ways by interaction with adsorbed oxygen or sodium atoms. Evidence for both local interactions and long range electronic effects is found.

500,485

PB86-132529

Not available NTIS

National Bureau of Standards, Gaithersburg, MD. Polymers Div.

Elastic Coherent Scattering from Multicomponent Systems. Applications to Homopolymer Mixtures and Copolymers.

Final rept.,

H. Benoit, W. Wu, M. Benmouna, B. Mozer, and B. Bauer. 1985, 8p

Pub. in Macromolecules 18, p986-993 1985.

Keywords: *Copolymers, *Elastic scattering, *Polymers, *Thermodynamics, Solutions, Polystyrene, Polymethyl methacrylate, Reprints, *Small angle scattering, Numerical solution.

A general equation giving the scattering intensity of a solution of polymers and copolymers at any concentration and angle is derived. Its relation with thermodynamics and its application to polydisperse systems are discussed. Small-angle neutron scattering experiments on a diblock copolymer of deuterated polystyrene-poly(methyl methacrylate)(PS-PMMA) were performed in bulk and in solution near the theta point. The results are consistent with the theoretical predictions.

500,486

PB86-132545

Not available NTIS

National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.

Decay Channels of the 3p Resonance in the 3d Transition Metals and Their Relevance to the Mechanism of Electron- and Photon-Stimulated Ion Desorption.

Final rept.,

E. Bertel, R. Stockbauer, R. L. Kurtz, T. E. Madey, and D. E. Ramaker. 1985, 8p

Sponsored by Office of Naval Research, Arlington, VA. Pub. in Surface Science 152/153, p776-783 1985.

Keywords: *Transition metals, *Molecular energy levels, *Chromium, Excitation, Oxygen, Ions, Reprints, *Photon stimulated ion desorption method, *Electron stimulated desorption, Oxygen ions.

The 3p excitation cross section in the 3d transition metals shows a resonant maximum in photoabsorption and electron energy loss spectroscopy. The resonant 3p excitation is shown to decay into various decay channels with Auger decay and direct recombination being most prominent. Electron and photon stimulated ion desorption from the 3d transition metal oxide surfaces is initiated by Auger induced 2 hole and 2 hole, 1 electron final states. In Cr(110)/O2 the O(+1) yield differs significantly from the total secondary electron yield. This rules out electron stimulated ion desorption induced by secondary electrons. It is the first instance of a pronounced core hole state sensitivity observed in PSD.

500,487

PB86-132552

Not available NTIS

National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.

Resonant Photoemission and the Mechanism of Photon-Stimulated Ion Desorption in a Transition-Metal Oxide.

Final rept.,

E. Bertel, R. Stockbauer, R. L. Kurtz, D. E. Ramaker, and T. E. Madey. 1985, 4p

Sponsored by Office of Naval Research, Arlington, VA. Pub. in Physical Review B: Condensed Matter 31, n8 p5580-5583, 15 Apr 85.

Keywords: *Transition metals, *Metal oxides, *Molecular energy levels, *Synchrotron radiation, *Chromium, Excitation, Photoemission, Ions, Reprints, *Photon stimulated ion desorption method, Oxygen ions.

The Cr 3p excitation spectrum has been studied in the Cr(110) surface oxide using synchrotron radiation in the photon-energy range 40-75 eV. The photon-stimulated-desorption O(+1) yield from the surface is seen to be sensitive to the electronic configuration of the Cr 3p core-hole state. The results are discussed in the context of the competitive decay processes which also depend on the electronic configuration of the 3p core-hole state.

500,488

PB86-132560

Not available NTIS

National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.

Photon-Stimulated Desorption of H(+s) Ions from OH on Ti and Cr: Comparison with Bulk Solid H2O.

Final rept.,

E. Bertel, D. E. Ramaker, R. L. Kurtz, R. Stockbauer, and T. E. Madey. 1985, 3p

Sponsored by Office of Naval Research, Arlington, VA. Pub. in Physical Review B: Condensed Matter 31, n10 p6840-6842, 15 May 85.

Keywords: Comparison, Excitation, Ions, Reprints, *Photon stimulated ion desorption method, *Hydrogen ions, Hydroxyl radicals.

An interpretation and comparison of photon-stimulated desorption yields of H(+1) ions from OH on Ti and Cr and from bulk solid H2O indicate that desorption occurs through two entirely different mechanisms. The first involves an intramolecular excitation of the OH adsorbate producing a H(+1) yield similar to that in bulk H2O. The second involves metal core-level excitation followed by Auger decay and is an example of molecular adsorbate dissociation arising from a metal-substrate Auger decay. This is a further generalization of the Knotek-Feibelman model applicable for desorption in ionic systems.

500,489

PB86-132578 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.

Electrochemical Noise Measurements for the Study of Localized Corrosion and Passivity Breakdown.

Final rept.,
U. Bertocci, J. L. Mullen, and Y. Ye. 1983, 6p
Pub. in Proceedings of Passivity of Metals and Semiconductors, Bombannes, France, May 30-June 3, 1983, p229-234.

Keywords: *Electrochemistry, *Corrosion, *Acoustic measurement, *Electrodes, *Passivity, Comparison, Aluminum, Chromium steels, Pitting.

Measurement of the random fluctuations of the current for Al, Fe-Cr and amorphous Fe-Ni-Cr electrodes are reported, both in the form of time records and frequency spectra. Comparison between the noise measured when no pitting could occur and when pitting was possible, showed that detectable fluctuations were present only in the second case. For the amorphous alloy, which is not susceptible to pitting, little noise could be measured even when the electrode was undergoing transpassive dissolution. Examples of random noise used for measuring electrode impedance are also given.

500,490

PB86-132586 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.

Examination of Current Fluctuations during Pit Initiation in Fe-Cr Alloys.

Final rept.,
U. Bertocci, and Y. Ye. 1984, 7p
Pub. in Jnl. of the Electrochemical Society 131, n5 p1011-1017 1984.

Keywords: *Chromium steels, *Passivity, *Pitting, *Electrochemistry, *Corrosion, *Acoustic measurement, Comparison, Reprints.

Random fluctuations of the passive current for Fe-Cr alloys of various Cr content have been examined, both in borate buffer and in the same solution with 0. mol/L NaCl added. Frequency spectra of these fluctuations have been recorded before and during pit initiation. No detectable fluctuations were observed in the absence of chlorides, when pitting does not occur. Comparison with the current noise measured before pit initiation indicates that the most important role of the aggressive ions is that of increasing the chance of local breakdown of the passive film. Frequency spectra give information concerning the time constants of the various processes, including repassivation. No correlation was found between the rate of attack during pitting and noise amplitude.

500,491

PB86-132636 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.

Interactions of Sulfur with Nickel Surfaces: Adsorption, Diffusion, and Desorption.

Final rept.,
M. Blaszczynski, R. Blaszczynski, R. Meclowski, A. J. Melmed, and T. E. Madey. 1983, 15p
Pub. in Surface Science 131, n2-3 p433-447 1983.

Keywords: *Surface chemistry, *Sulfur, *Adsorption, *Diffusion, *Desorption, Nickel, Emission spectroscopy, Reprints.

The kinetics of adsorption, surface diffusion and thermal desorption of sulfur on Ni surfaces, have been studied using field electron emission microscopy methods. The sticking probability for elementary sulfur sublimed onto a Ni specimen is approximately unity for Ni substrate temperatures from 77 to 530 K. For multilayer adsorption of sulfur, diffusion occurs without motion of a sharp boundary, and there is evidence of extensive surface reaction between S and Ni (emission from small 'crystallites' is evident in the field emission patterns). Sulfur desorbs from Ni at temperatures above 1500 K.

500,492

PB86-133352 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Inorganic Materials Div.

Environmental Inorganic Chemistry of Main Group Elements with Special Emphasis on Their Occurrence as Methyl Derivatives.

Final rept.,
F. E. Brinckman. 1985, 44p
Pub. in Proceedings of U.S. - Italy Joint Seminar and Workshop on Environmental Inorganic Chemistry, San Miniato, Italy, June 5-10, 1983, Environmental Inorganic Chemistry, p195-238 1985.

Keywords: *Environmental surveys, *Inorganic compounds, *Methanes, *Metal containing organic compounds, Reaction kinetics, Reviews, Geochemistry, Chemical reactions, Metabolism, Surface chemistry, Membranes, Transport properties, Comparison, *Clathrate compounds, Bioaccumulation, Path of pollutants, Natural emissions.

Deposition, relocation, transformations, biological uptake, and metabolism are among major kinds of information available for organic molecules in the environment, whether toxic or essential. Present-day information for comparable processes of metals and metalloids in environmental media in terms of their molecular processes lags far behind, though almost all Main Group elements play a crucial role in living organisms and geochemistry. The review emphasizes inorganic studies, many drawn from classical examples, as aids to surveying recent contributions to the environmental chemistry of Main Group metals and metalloids. Selected topics, including transmethylation kinetics, photomethylation, direct surface reactions, membrane attachment and lipophilicity, and naturally-occurring organometalloids and organo-metals, are discussed as a means to illustrate future needs and prospects in the field. The relationships between purely inorganic molecular species and their more labile methyl derivatives provides a useful range of comparisons, based upon over 150 references.

500,493

PB86-133394 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Center for Materials Science.

Comment on 'New Critical Point in the Vicinity of the Freezing Temperature of Potassium-Cesium (K₂Cs)'.

Final rept.,
J. W. Cahn, and J. L. Murray. 1983, 1p
Pub. in Physical Review Letters 51, n16 p1493 1983.

Keywords: *Critical point, *Freezing, *Cesium alloys, *Potassium alloys, Phase diagrams, Calorimetry, Heat capacity.

A recent report of a critical point in the K-Cs system seemed unlikely to the authors. With the existing phase diagram and calorimetric data the authors could fit quite accurately almost all the data including those that led to the hypothesized critical point. The only discrepancy was resolved when they contacted the author and found that a power outage had occurred which they had not deemed significant enough to report. They conclude that no change in the phase diagram is needed to account for these data.

500,494

PB86-133402 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.

Nonequilibrium Surface and Interface Thermodynamics.

Final rept.,
J. W. Cahn. 1983, 5p
Pub. in Proceedings of NATO Advanced Research Institute on Atomistics of Fracture, Calcatoggio, Corsica, France, May 22-31, 1981, Atomistics of Fracture, p427-431 1983.

Keywords: *Surface chemistry, *Thermodynamics, *Adsorption, *Fractures(Materials).

Thermodynamics of surfaces has played an important role in the development of fracture criteria. It seems clear that many of these classical papers were based on simplifying assumptions whose validity needs to be reexamined. The recent concerns with the subtleties of the effects of adsorption underscore this point. The difficulty of finding and proving the validity of simple inequalities for surface creation in nonequilibrium systems and Gibbs' counterexample should serve as warning that these concerns are real and deserve our attention.

500,495

PB86-133451 Not available NTIS

National Bureau of Standards (NML), Gaithersburg, MD. Molecular Spectroscopy Div.

Time-Resolved Measurements of Vibrational Relaxation of Molecules on Surfaces: Hydroxyl Groups on Silica Surfaces.

Final rept.,
M. P. Casassa, E. J. Heilweil, J. C. Stephenson, and R. R. Cavanagh. 1985, 2p
Sponsored by Air Force Office of Scientific Research, Bolling AFB, DC.
Pub. in Jnl. of Vacuum Science and Technology A3, n3 p1655-1656 May/Jun 85.

Keywords: *Molecular relaxation, *Molecular vibration, *Silicon dioxide, *Surface chemistry, Infrared spectroscopy, Reprints, *Hydroxyl radicals.

The vibrational population relaxation rate of the O-H stretching fundamental of hydroxyl groups on SiO₂ surfaces was measured directly using picosecond infrared pulses. The vibrational lifetime determined for hydroxyls at the silica-vacuum interface is 204 + or - 20 ps. For silica-bound hydroxyls in a saturated atmosphere of CCl₄, the lifetime decreases to 159 + or - 16 ps. Both lifetimes are many times longer than would be inferred from infrared absorption linewidths.

500,496

PB86-133477 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Molecular Spectroscopy Div.

Laser Studies of Surface Chemical Reactions.

Final rept.,
R. R. Cavanagh, and D. S. King. 1984, 18p
Pub. in Springer Series of Chemical Physics 35, n5 p141-158 1984.

Keywords: *Surface chemistry, *Nitrogen oxide(NO), *Desorption, *Fluorescence, Dynamics, Doppler effects, Molecular energy levels, Ruthenium, Oxidation, Angular distribution, Reprints, *Laser excited fluorescence.

A review of laser studies of surface chemical dynamics with emphasis on thermal desorption processes is presented. The correlation of gas phase and liquid molecular dynamics with analogous surface processes is demonstrated, with primary emphasis on experimental techniques for monitoring relevant quantum state populations. Recent results for the desorption of NO from Ru(001) and NO from oxidized Ru crystals are compared in terms of rotational populations, and velocity and angular flux distributions.

500,497

PB86-133485 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Thermophysics Div.

Heat Capacity and Electrical Resistivity of POCO AXM-5Q1 Graphite in the Range 1500-3000 K by a Pulse-Heating Technique.

Final rept.,
A. Cezairliyan, and A. P. Müller. 1985, 16p
Sponsored by Air Force Office of Scientific Research, Bolling AFB, DC.
Pub. in International Jnl. of Thermophysics 6, n3 p285-300 May 85.

Keywords: *Graphite, *Specific heat, *Electrical resistivity, High temperature tests, Pulse heating, Reprints.

Measurements of the heat capacity and electrical resistivity of POCO AXM-5Q1 graphite in the temperature range 1500-3000 K by a subsecond-duration pulse-heating technique are described.

500,498

PB86-133519 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Thermophysics Div.

Leung-Griffiths Model for the Thermodynamic Properties of the Mixture of Carbon Dioxide and Ethane Near the Gas-Liquid Critical Line.

Final rept.,
R. F. Chang, and T. Doiron. 1983, 16p
Pub. in International Jnl. of Thermophysics 4, n4 p337-352 1983.

Keywords: *Mathematical models, *Carbon dioxide, *Ethane, *Phase transformation, Thermodynamic properties, Equations of state, Mixtures, Critical points, Comparison, Reprints, Numerical solution.

Leung and Griffiths have proposed a thermodynamic fundamental equation for a binary mixture near the crit-

Field 7—CHEMISTRY

Group 7D—Physical Chemistry

ical line. The equation is of the scaling form which incorporates nonclassical exponents. They developed the equation based on the idea that the thermodynamic properties of mixtures can be obtained from the interpolation between the critical properties of pure components when a set of suitable variables are used. They demonstrated the applicability of the idea successfully in the mixture of He3 and He4 in which the critical line is a nearly linear function of composition. We have used a Leung-Griffiths type equation of state to describe the thermodynamic properties of the mixture of carbon dioxide and ethane. The critical line of this mixture is, unlike that of He3 and He4, a non-linear function of composition and the azeotropic line extends to the critical line. Comparison of the predictions of the equation to experimental data shows a good agreement for the mixtures of CO2 and C2H6.

500,499

PB86-133568

Not available NTIS
National Bureau of Standards, Gaithersburg, MD.

Electric Field Effects on the Absorption Spectra of Molecular Hydrogen Near the Ionization Limit.

Final rept.,

J. W. Cooper, E. B. Saloman, B. E. Cole, and 1983, 3p

Pub. in *Physical Review A: General Physics* 28, n3 p1832-1834 1983.

Keywords: *Hydrogen, *Photoionization, *Ultraviolet spectroscopy, *Absorption spectra, Stark effect, Electric fields, Reprints.

The absorption cross section of H2 has been measured in the region between 77.5 and 83.7 micrometers and the effects of electric fields up to 22 kV/cm on the cross sections has been investigated. The apparent cross section is found to be increased in the neighborhood of optically allowed transitions to ν rho sigma and ν rho pi states with $\nu=4-7$. This increase in absorption is attributed to field mixing with nearby optically forbidden states.

500,500

PB86-133824

Not available NTIS
National Bureau of Standards, Gaithersburg, MD.

Reaction of Oxygen Atoms with Olefins.

Final rept.,

R. J. Cvetanovic, and D. L. Singleton. 1984, 44p

Pub. in *Rev. Chem. Intermed.* 5, n2 p183-226 1984.

Keywords: *Reaction kinetics, *Alkene hydrocarbons, Chemical reactions, Atomic energy levels, Reprints, *Chemical reaction mechanisms, *Oxygen atoms.

The mechanisms and kinetics of the chemical reactions of the ground state oxygen atoms, O(triplet P), with olefins are reviewed in detail. More recent experimental and theoretical literature is analyzed with respect to its bearing on the early pioneering and extensive subsequent developments in this field carried out in authors' laboratory.

500,501

PB86-133832

Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.

Ni/Cr Interface Width Dependence on Sputtered Depth.

Final rept.,

F. Davarya, M. L. Roush, J. Fine, T. D. Andreadis, and O. F. Goktepe. 1983, 4p

Jnl. of Vacuum Science and Technology A-Vacuum Surfaces and Films 1, n2 p467-470 1983.

Keywords: *Interfaces, *Thin films, *Topography, *Nickel, *Chromium, Monte Carlo methods, Auger electrons, Sputtering, Reprints.

The composition depth distribution of an interface as determined by Auger sputter depth profiling is dependent, to a large extent, on both the ion bombardment induced cascade mixing and on the surface topography generated as a result of ion erosion. The authors assess the relative influence of these two processes on the depth resolution by comparing interface widths obtained by Auger sputter depth profiling (resulting from both the cascade mixing and the topography) to interface widths obtained by computer simulation (due to cascade mixing alone). Depth profiles were measured at eight successive interfaces of a multilayered Ni/Cr/Ni/Cr...thin-film structure using both 1 and 3-keV argon ion beams for sputter profiling. These interface widths increase with sputter depth, the increase being more rapid for the 3-keV bombardment. The calculations with the computer code EVOLVE contain

modeling of all contributions to interface broadening except that of surface topography, thus resulting in constant values of interface widths. The difference in width obtained from the measured and calculated data is used to estimate the extent of the topography produced as a function of sputtered depth.

500,502

PB86-136744

Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.

Photoionization Dynamics of Small Molecules.

Final rept.,

J. L. Dehmer, D. Dill, and A. C. Parr. 1985, 68p

Pub. in *NATO ASI Ser., Ser. C, Photophys. Photochem. Vac. Ultraviolet* 142, p341-408 1985.

Keywords: *Photochemical reactions, *Ionization, *Dynamics, Excitation, Reprints, *Autoionization.

Photoionization dynamics of small molecules are discussed with emphasis on shape and autoionizing resonances. These resonant processes are important probes of the photoionization process for various reasons, the most obvious one being that they are usually displayed prominently against nonresonant behavior in such observables as the total photoionization cross section, photoionization branching ratios, and photoelectron angular distributions. More importantly, the study of these resonant features has repeatedly led to a deeper physical insight into the mechanisms of excitation, resonant trapping of the photoelectron, and decay of the excited complex that occur during the photoionization process. Of particular interest in this context are the uniquely molecular aspects resulting from the anisotropic molecular field and the interplay among rovibronic modes. The authors review the fundamental aspects of both types of resonant process and discuss recent progress and prospects for future work from both experimental and theoretical points of view. Finally, a brief overview of various approaches not covered in the main discussion is presented to stress the variety of complementarity of alternative probes of molecular photoionization dynamics.

500,503

PB86-136751

Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Center for Chemical Physics.

Aqueous Solubilities and Enthalpies of Solution of Adenine and Guanine.

Final rept.,

H. DeVoe, and S. P. Wasik. 1984, 10p

Pub. in *Jnl. of Solution Chemistry* 13, n1 p51-60 1984.

Keywords: *Solubility, *Enthalpy, *Adenine, *Guanine, Solutions, Temperature, Reprints, Liquid chromatography.

A generator column - liquid chromatographic technique was used to determine the aqueous solubility of adenine in the temperature range 20 - 30 C, and of guanine in the range 15 - 40 C. The adenine enthalpy value includes a small correction for association in the saturated solutions. The previously undetermined molar enthalpy of the second ionization step of guanine (to form the doubly-charged guanine anion) is estimated from our data combined with other measurements to equal (33.8 ± 2.9) kJ/mol.

500,504

PB86-136777

Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.

Radiation-Induced Formation of Thymine-Thymine Crosslinks.

Final rept.,

M. Dizdareglu, and M. G. Simic. 1984, 6p

Pub. in *International Jnl. of Radiation Biology and Related Studies in Physics, Chemistry and Medicine* 46, n3 p241-246 1984.

Keywords: *Dimers, *Radiation effects, Crosslinking, Gas chromatography, Reprints, *Thymine, *Hydroxyl radicals, Chemical reaction mechanisms.

The formation of thymine dimers as a major consequence of radiation-generated OH radical reactions with thymine in aqueous solutions is reported. About one half of the intermediates which resulted from OH reactions with thymine, i.e., thymine radicals, dimerize, indicating dimerization as one of the major reaction pathways. The other half of thymine radicals disproportionate and give previously observed monomeric products. One should point out that the 'thymine dimers' observed in this work are not the same as the UV light-induced dimers of thymine.

500,505

PB86-136793

Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.

Orientational Ordering of an Incommensurate Sodium Layer on Ru(001).

Final rept.,

D. L. Doering, and S. Semancik. 1984, 1p

Pub. in *Jnl. of Vacuum Science and Technology A-Vacuum Surfaces and Films* 2, n2 p893 1984.

Keywords: *Surface chemistry, *Sodium, *Chemisorption, Ruthenium, Orientation, Reprints, *Low energy electron diffraction.

Orientational ordering refers to the azimuthal alignment of an overlayer into a specific orientation relative to a substrate lattice. Experimental demonstrations of this effect for solid, incommensurate monolayers have been reported previously for inert gases physisorbed on graphite. The work summarized here describes the first detailed examination of orientational ordering in a strongly chemisorbed incommensurate layer.

500,506

PB86-136876

Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.

Core-Level Binding-Energy Shift Analysis of Adsorption and Dissociation.

Final rept.,

W. F. Egelhoff. 1984, 3p

Pub. in *Physical Review B: Condensed Matter* 29, n6 p3681-3683 1984.

Keywords: *Adsorption, *Dissociation, *Thermochemistry, Atomic energy levels, Molecular energy levels, Photoemission, Nitrogen, Nitrogen oxides(NO), Reprints.

An analysis of core-level binding-energy shifts of adsorbed atoms and molecules is used to determine important thermochemical quantities which are often otherwise unmeasurable. Also presented are a new approach to interpreting adsorbate core-level spectra and a novel technique for probing adsorbed molecules in energetically unfavored orientations.

500,507

PB86-136884

Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.

Surface Electronic-Structure Changes Induced by Chemisorption. Summary Abstract.

Final rept.,

W. F. Egelhoff. 1984, 2p

Pub. in *Jnl. of Vacuum Science and Technology A-Vacuum Surfaces and Films* 2, n2 p932-933 1984.

Keywords: *Nickel, *Chemisorption, *Surfaces, Carbon monoxide, Adsorption, Reprints, *Electronic structure, X ray photoelectron spectroscopy.

X-ray photoelectron spectroscopy has been used to study the changes in the electronic structure of Ni(100) surface Ni atoms when carbon monoxide is adsorbed. The basic trends are for the d-shell to fill up and for the s-shell to empty. This produces a Ni configuration of approximately $3(d \text{ sup } 10) 4(s \text{ sup } 0)$.

500,508

PB86-136892

Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.

Core-Level Binding-Energy Shift Analysis of N2 on Ni(100). Summary Abstract.

Final rept.,

W. F. Egelhoff. 1984, 1p

Pub. in *Jnl. of Vacuum Science and Technology A-Vacuum Surfaces and Films* 2, n2 p1013 1984.

Keywords: *Molecular energy levels, *X ray analysis, *Surface chemistry, *Nickel, *Thermochemistry, X ray spectroscopy, Photoemission, Atomic energy levels, Nitrogen, Nitrogen oxide(NO), Reprints.

The equivalent core approximation has been used together with a Born-Haber cycle analysis to treat the x-ray photoelectron spectra of the nitrogen 1s core levels of molecular N2 adsorbed on the Ni(100) surface. The analysis yields the heats of adsorption of nitric oxide, oxygen atom down and nitrogen atom down.

500,509

PB86-136900 Not available NTIS
National Bureau of Standards (NML), Gaithersburg,
MD. Surface Science Div.

Core-Level Binding-Energy Shift Analysis of CO, H, and O Adsorption on Cu-Ni Surfaces.

Final rept.,
W. F. Egelhoff. 1985, 4p
Pub. in Jnl. of Vacuum Science and Technology A3, n3
p1305-1308 May/June 85.

Keywords: *Carbon monoxide, *Hydrogen, *Oxygen, *Adsorption, *Molecular energy levels, *Surface chemistry, Copper, Nickel, Desorption, Chemisorption, Thermochemistry, Reprints.

The equivalent core approximation ($Z + 1$) is used with a Born-Haber cycle analysis to analyze the Ni2p(sub 3/2) surface core-level binding-energy shifts which occur upon adsorption of CO, H, and O on Ni(100). The analysis gives values for the heats of desorption of these gases from Cu-Ni alloy surfaces. Perhaps more importantly, it also provides a quantitative determination of how chemisorption of CO, H, and O modify the heats of surface segregation for Cu-Ni surfaces.

500,510

PB86-136942 Not available NTIS
National Bureau of Standards (NML), Gaithersburg,
MD. Surface Science Div.

N2 on Ni(100): Angular Dependence of the N(sub 1s) XPS (X-ray Photoelectron Spectroscopy) Peaks.

Final rept.,
W. F. Egelhoff. 1984, 5p
Pub. in Surface Science 141, pL324-L328 1984.

Keywords: *X ray spectroscopy, *Nickel, *Surface chemistry, *Adsorption, Nitrogen, Molecular structure, Reprints, Nitrogen atoms.

The X-ray photoelectron spectrum of molecular N₂ adsorbed in a c(2x2) structure on Ni(100) shows two N(sub 1s) peaks in the fully-screened N(sub 1s) region around 400 eV binding energy and a shake-up structure around 405 eV. The assignment of the two fully-screened peaks to the two inequivalent N atoms is established on the basis of the angular variation in the peak intensities. This assignment provides important support for a Born-Haber cycle analysis of these peaks.

500,511

PB86-137627 PC A04/MF A01
National Bureau of Standards, Gaithersburg, MD.
Journal of Research of the National Bureau of Standards, Volume 90, Number 4, July-August 1985.

Aug 85, 69p
See also PB86-137635 through PB86-137676, and PB85-237329. Also available from Supt. of Docs as SN703-027-000005-9.

Keywords: *Research projects, Calibrating, Density(Mass/volume), Comparison, Silicon, Standards, Enthalpy, Combustion, Triazines, Calorimeters, Corrosion, Bioassay, Deoxyribonucleic acids, Rydberg series, Computer applications.

Contents:

- Recalibration of the U.S. National Prototype Kilogram;
- Density comparison of silicon artifacts between NML (Australia) and NBS (U.S.);
- Mass comparator for in-situ calibration of large mass standards;
- Determination of the enthalpies of combustion and formation of substituted triazines in an adiabatic rotating bomb calorimeter;
- Metrics and techniques to measure microcomputer productivity;
- Field effects on Rydberg atoms;
- International assembly discusses mechanisms of DNA damage repair;
- Microbes play a considerable role in corrosion.

500,512

PB86-137932 Not available NTIS
National Bureau of Standards (NML), Boulder, CO.
Quantum Physics Div.

Correlation Effects of a Phase-Diffusing Field on Two-Photon Absorption.

Final rept.,
D. S. Elliott, M. W. Hamilton, K. Arnett, and S. J. Smith. 1985, 9p
Sponsored by Department of Energy, Washington, DC.
Pub. in Physical Review A: General Physics 32, n2
p887-895 Aug 85.

Keywords: Reprints, *Two photon absorption, *Sodium atoms, Laser radiation.

Experimental evidence of field-correlation effects on weak-field two-photon absorption in atomic sodium is presented. In the case of a nearly Lorentzian laser power spectrum, the absorption profile has four times the spectral width of the exciting field, in agreement with predictions by Mollow. The measurement is carried out with counterpropagating laser beams to cancel Doppler broadening. The width of the two-photon absorption spectrum is decreased by partially decorrelating the counterpropagating laser beams. Increasing the correlation time of the frequency fluctuations, resulting in a nearly Gaussian laser power spectrum, has also been observed to decrease the width of the absorption spectrum. An extension of the time-dependent second-order perturbation theory to these additional cases yields good agreement.

500,513

PB86-137965 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.

Determination of Longitudinal Crystal Moduli in Polymers by Spectroscopic Methods.

Final rept.,
B. Fanconi, and J. F. Rabolt. 1985, 15p
Pub. in Jnl. of Polymer Science: Polymer Physics Edition 23, p1201-1215 1985.

Keywords: *X ray diffraction, *Polymers, *Raman spectroscopy, *Modulus of elasticity, Inelastic scattering, Neutron scattering, Reprints, Numerical solution.

Experimental methods for determining longitudinal crystal moduli of polymers were evaluated in light of recent processing methods that produced macroscopic Young's moduli which exceeded ultimate values as found by the x-ray diffraction method. The spectroscopic techniques of Raman and coherent inelastic neutron scattering yielded higher longitudinal crystal moduli than x-ray diffraction, and from calculations described herein it is concluded that these spectroscopic values are better estimates of the maximum Young's moduli in fully aligned and crystalline polymeric materials.

500,514

PB86-137973 Not available NTIS
National Bureau of Standards (NML), Gaithersburg,
MD. Surface Science Div.

Ammonia Adsorption on the Ag(311) Surface.

Final rept.,
S. T. Ceyer, and J. T. Yates. 1985, 12p
Pub. in Surface Science 155, p584-595 1985.

Keywords: *Silver, *Surface chemistry, *Adsorption, Molecular structure, Chemical bonds, Ammonia, Performance evaluation, Reprints, Electron stimulated desorption ion angular distribution method, Thermal desorption spectroscopy, Electron energy loss spectroscopy.

The adsorption of ammonia on the Ag(311) surface has been studied by ESDIAD (electron stimulated desorption-ion angular distributions), high resolution electron energy loss spectroscopy and thermal desorption spectroscopy. Two desorption peaks are observed in the thermal desorption spectra and are correlated with two bonding geometries. The more strongly bound state corresponds to ammonia bound on top of the ridge atom through the nitrogen end with its C(sub 3v) axis perpendicular to the macroscopic surface. It is suggested that the less strongly bound state corresponds to ammonia molecules lying down in the troughs.

500,515

PB86-138054 Not available NTIS
National Bureau of Standards (NML), Gaithersburg,
MD. Surface Science Div.

Kinetics of Sputter-Enhanced Surface Segregation at a Ni/Ag Interface.

Final rept.,
J. Fine, T. D. Andreadis, and F. Davarya. 1983, 2p
Pub. in Jnl. of Vacuum Science and Technology A-Vacuum Surface and Films 1, n2 p507-508 1983.

Keywords: *Sputtering, *Nickel, *Silver, *Ion beams, *Ion irradiation, Reaction kinetics, Diffusion, Surfaces, Reprints, *Auger spectroscopy.

Sputter profiling of a Ni/Ag interface produces a mixed Ni-Ag surface region and the authors have found that in such a region that Ag will segregate to the surface. This segregation can be observed to occur in real time after the ion bombardment has been stopped. Auger spectroscopy was used to obtain a unique set of measurements of the kinetics of surface segregation due to bombardment enhanced diffusion and to determine the thickness of the segregated Ag layer at equilibrium.

500,516

PB86-138088 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Laser Desorption Mass Spectrometry of Surface-Absorbed Molecules.

Final rept.,
R. A. Fletcher, I. Chabay, D. A. Weitz, and J. C. Chung. 1984, 5p
Pub. in Chemical Physics Letters 104, n6 p615-619 1984.

Keywords: *Mass spectroscopy, *Surface chemistry, *Adsorption, Desorption, Visible spectroscopy, Ultraviolet spectroscopy, Reprints, *Laser spectroscopy, *Time of flight mass spectroscopy.

The role of surface microstructure in the visible and UV pulsed laser desorption of surface adsorbates is examined. It is shown that the surface roughness aids in a relatively gentle thermal desorption of adsorbed molecular monolayers, substantially increasing the sensitivity and selectivity of time of flight mass spectroscopy in the analysis of adsorbates on metal surfaces.

500,517

PB86-138138 Not available NTIS
National Bureau of Standards (NEL), Boulder, CO.
Thermophysical Properties Div.

Thermal-Conductivity Enhancement Near the Liquid-Vapor Critical Line of Binary Methane-Ethane Mixtures.

Final rept.,
D. G. Friend, and H. M. Roder. 1985, 4p
Pub. in Physical Review A: General Physics 32, n3
p1941-1944 Sep 85.

Keywords: *Thermal conductivity, *Critical point, *Binary systems(Materials), *Methane, *Ethane, Mixtures, Alkanes, Liquid phases, Vapor phases, Temperature, Reprints.

Measurements of the thermal conductivity of mixtures of methane and ethane reveal an enhancement in the mixture critical region apparently contradicting theoretical predictions. The anomaly is similar in size and temperature dependence to that found for pure fluids.

500,518

PB86-138146 Not available NTIS
National Bureau of Standards (NML), Gaithersburg,
MD. Radiation Physics Div.

Hydroxyl Radical-Induced Crosslinks of Methionine Peptides.

Final rept.,
E. Gajewski, M. Dizdargolu, H. C. Krutzsch, and M. G. Simic. 1984, 9p
Sponsored by National Cancer Inst., Bethesda, MD.
Pub. in International Jnl. of Radiation Biology and Related Studies in Physics, Chemistry and Medicine 46, n1 p47-55 1984.

Keywords: *Peptides, Crosslinking, Gas chromatography, Mass spectroscopy, Hydrolysis, Samples, Reprints, *Hydroxyl radicals, *Methionine, *Methionines, Dimers, Homocysteine, Butanic acid/amino-(methyl-dithio), Butanoic acid/thiobis(amino).

Reactions of radiation-generated OH radicals with methionine (Met) and its homopeptides, L-Met-L-Met and tri-L-Met, were investigated through reaction products. Samples of irradiated Met and HCl-hydrolyzates of its irradiated homopeptides were trimethylsilylated and analyzed by capillary gas chromatography-mass spectrometry. Mass spectra taken revealed the formation of three dimerization products, e.g., 2-amino-4-(methylthio)butanoic acid, 4,4'-thiobis(2-aminobutanoic acid) and homocysteine. G-values of these products were determined to be 0.1, 0.16 and 0.3, respectively.

Field 7—CHEMISTRY

Group 7D—Physical Chemistry

500,519

PB86-138153 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Chemical Thermodynamics Div.

Thermodynamics of the Conversion of Fumarate to L-(-)-Malate.

Final rept.,
E. Gajewski, R. N. Goldberg, and D. K. Steckler.
1985, 9p
Pub. in Biophysical Chemistry 22, p187-195 1985.

Keywords: *Thermodynamics, *Malates, Gas chromatography, Calorimetry, Enthalpy, Heat capacity, Enzymes, Catalysis, Chemical equilibrium, Fumarates, pH, Gibbs free energy, Reprints.

The thermodynamics of the conversion of aqueous fumarate to L-(-)-malate has been investigated using both heat conduction microcalorimetry and a gas chromatographic method for determining equilibrium constants. The reaction was carried out in aqueous Tris-HCl buffer over the pH range 6.3-8.0, the temperature range 25-47°C, and at ionic strengths varying from 0.0005 to 0.62 mol/kg. Equations are given which allow one to calculate the combined effects of pH and temperature on equilibrium constants and enthalpies of this reaction.

500,520

PB86-138187 Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.

Separated-Atom Theory of Laser-Induced Collisional Ionization of Cs by Sr.

Final rept.,
S. Geltman. 1982, 19p
Pub. in Photon-Assisted Collisions and Related Topics, p35-53 1982.

Keywords: *Cesium, *Ionization, Perturbation theory, Stark effect, *Atom molecule collision, *Laser induced ionization, *Strontium atoms.

A semiquantitative theoretical description is given for the observed laser-induced collisional ionization (LICI) of Cs by Sr atoms. This is done in the separated-atom picture in which the resonant interaction of the atoms with the radiation is fully taken into account and the collision is treated perturbatively. The basic intensity dependence of the cross section and its spectral width are well explained, but the distinctive observed line asymmetry is accounted for only qualitatively.

500,521

PB86-138203 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Inorganic Analytical Research Div.

Isotopic Variations in Commercial High-Purity Gallium.

Final rept.,
J. W. Gramlich, and L. A. Machlan. 1985, 3p
Pub. in Analytical Chemistry 57, n8 p1788-1790 1985.

Keywords: *Gallium isotopes, *Mass spectroscopy, Purity, Sampling, Reprints, *Thermal ionization mass spectroscopy, Atomic weights.

The relative isotopic composition has been determined in 16 samples of gallium metal using highly precise thermal ionization mass spectrometry. The results show variations in the $^{69}\text{Ga}/^{71}\text{Ga}$ ratio of up to 0.3% for the samples measured.

500,522

PB86-138229 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymer Science and Standards Div.

Monte Carlo Modeling of Kinetics of Polymer Crystal Growth: Regime III and Its Implications on Chain Morphology.

Final rept.,
C. M. Guttman, and E. A. DiMarzio. 1983, 13p
Pub. in Jnl. of Applied Physics 54, n10 p5541-5553 Oct 83.

Keywords: *Mathematical models, *Crystal growth, *Monte Carlo method, Crystallization, Reprints, *Polymer chains.

A Monte Carlo simulation of polymer crystal growth from the melt is presented. This two dimensional model approximates growth by laying down crystal stems one at a time. The Monte Carlo simulation of various geometric models of the crystal surface yields Regime I and Regime II growth similar to that predicted

by Lauritzen and Frank. The analytical expression of Frank is shown to be accurate. A recent prediction by Hoffman of a low temperature region (Regime III) with properties similar to Regime I has been verified. Regime III is lattice dependent. Specifically the solid on solid model (SOS) commonly used to model monatomic systems yields Regime III but is not space filling. The hexagonal lattice yields correctly formed crystals but does not show Regime III as long as we require that the crystals grow on one plane. On the hexagonal lattice, if we allow growth on more than one growth plane, we obtain both space filling crystals and Regime III growth. There are no regimes of growth other than the three discussed here.

500,523

PB86-138237 Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.

Product Vibrational State Distributions of Thermal Energy Charge Transfer Reactions Determined by Laser-Induced Fluorescence in a Flowing Afterglow: $\text{Ar}(+1) + \text{CO}$ yields $\text{CO}(+1)$ ($\nu=0-6$) + Ar.

Final rept.,
C. E. Hamilton, V. M. Bierbaum, and S. R. Leone.
1985, 9p
Sponsored by Air Force Office of Scientific Research, Bolling AFB, DC.
Pub. in Jnl. of Chemical Physics 83, n5 p2284-2292, 1 Sep 85.

Keywords: *Carbon monoxide, *Dynamics, *Molecular vibration, Afterglows, Reprints, *Ion molecule interactions, *Laser induced fluorescence.

The $\text{Ar}(+1) + \text{CO}$ yield $\text{CO}(+1)(\nu=0-6) + \text{Ar}$ charge transfer reaction is studied at thermal energy in a flowing afterglow and the vibrational state distribution is determined by laser-induced fluorescence on the $\text{CO}(+1)(A \text{ (sup } 2) \pi\text{-X(sup } 2) \sigma(+1) \text{ bands})$. The $\text{Ar}(+1) + \text{CO}$ reaction is described as proceeding via a bent $\text{ArCO}(+1)$ intermediate that forms in a side-on attack. Vibrational excitation may then result from delocalization of the bonding electron density of CO and the corresponding dynamical changes in the CO bond length in the intermediate.

500,524

PB86-138369 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.

Repair of Tryptophan Radicals by Antioxidants.

Final rept.,
S. V. Jovanovic, and M. G. Simic. 1985, 5p
Pub. in Jnl. of Free Radicals in Biology and Medicine 1, n2 p125-129 1985.

Keywords: *Free radicals, *Antioxidants, Proteins, Oxidation, Phenols, Ascorbic acid, Reprints, *Tryptophan radicals, Phenylene diamine N-N-N-N-tetramethyl-(dihydrochloride).

Oxidizing free radicals with redox potential greater than 1 V generate indole radicals as in tryptophan. These resonance-stabilized free radicals can be repaired efficiently with electron donors such as ascorbate, N,N,N1,N1-tetramethyl- p-phenylenediamine dihydrochloride (TMPD), and phenolic antioxidants.

500,525

PB86-138393 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Thermophysics Div.

Reaction Diffusion in a Medium Containing a Random Distribution of Nonoverlapping Traps.

Final rept.,
R. F. Kayser, and J. B. Hubbard. 1984, 4p
Pub. in Jnl. of Chemical Physics 80, n3 p1127-1130 1984.

Keywords: *Reaction kinetics, *Diffusion, *Traps, Density(Mass/volume), Random functions, Reprints.

The transient reaction-diffusion kinetics in a system containing a random distribution of stationary spherical traps is analyzed. It is shown that recently obtained results concerning the long-time behavior of the trap-averaged density at the origin, may be readily extended to the cases of partially absorbing and non-overlapping traps, independently of the number density of traps. The authors also estimate the size of the relative fluctuations and show that these fluctuations diverge at long times.

500,526

PB86-138401

Not available NTIS

National Bureau of Standards (NEL), Gaithersburg, MD. Thermophysics Div.

Diffusion In a Medium with a Random Distribution of Static Traps.

Final rept.,
R. F. Kayser, and J. B. Hubbard. 1983, 4p
Pub. in Physical Review Letters 51, n2 p79-82, 11 Jul 83.

Keywords: *Reaction kinetics, *Diffusion, *Traps, Density(Mass/volume), Random functions, Reprints.

The authors consider particles diffusing in d-dimensional space among a random distribution of stationary spherical traps. Given a particle at the origin at time $t=0$, they show that the density of particles at the origin as t goes to infinity must decay at least as fast as $(-t(\text{sub } d/(d+2)))$. The density here is obtained by averaging the diffusive field for a given configuration of traps over all configurations. The upper bound coincides with the lower bound recently derived by Grassberger and Procaccia.

500,527

PB86-138419 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.

Concentration Dependence of the Diffusion Coefficient and the Longest Relaxation Time of Polymer Chains in Solution.

Final rept.,
D. E. Kranbuehl, and P. H. Verdier. 1985, 3p
Sponsored by American Chemical Society, Washington, DC.
Pub. in Macromolecules 18, n8 p1638-1640 1985.

Keywords: *Diffusion, *Molecular relaxation, *Dynamics, *Mathematical models, *Polymers, Solutions, Monte Carlo method, Concentration(Composition), Reprints, *Polymer chains.

The concentration dependence of the translational diffusion constant of polymer chains in non-dilute solutions has been examined by direct computer simulation for simple lattice-model chains. In agreement with several recent experimental studies, the results show no sign of regions of constant power-law dependence of diffusion constant upon concentration predicted by some theoretical models. They also appear to suggest that the major part of the concentration dependence may be accounted for by simple free-volume considerations.

500,528

PB86-138435 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymer Science and Standards Div.

Time Dependence of Mechanical and Transport Properties of Drawn and Annealed Linear Polyethylene.

Final rept.,
F. Decandia, V. Vittoria, and A. Peterlin. 1985, 18p
Sponsored by Consiglio Nazionale delle Ricerche, Milan (Italy).
Pub. in Jnl. of Polymer Science, Polymer Physics Edition 23, p1217-1234 1985.

Keywords: *Polyethylene, *Mechanical properties, *Transport properties, Polymers, Reprints, *Crystalline polymers.

Linear polyethylene both as drawn, or drawn and subsequently annealed with free ends, changes its length, density, crystallinity, elastic modulus, sorption, and diffusivity as the sample stands completely unrestrained at room temperature. Most of these changes occur during the first few hours. But they are important on a molecular scale since they suggest strongly that drawn, and drawn and annealed samples are far from equilibrium. As a consequence of the tendency of each mobile tie molecule in the amorphous conformation to retract and to crystallize, the specimen approaches but does not reach complete equilibrium. The transient seems to be caused by slow crystallization of tie molecules which creates crystalline bridges across the amorphous layers.

500,529

PB86-138443 Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.

Effect of Spin-Orbit Excitation on Chemical Reactivity: Laser Transient Absorption Spectroscopy of Br(doublet P(1/2), doublet P(3/2)) + IBr Reactive Dynamics.

Final rept.,
H. K. Haugen, E. Weitz, and S. R. Leone. 1985, 8p
Grants NSF-CHE79-11340, NSF-PHY82-00805
Sponsored by National Aeronautics and Space Administration, Washington, DC., and National Science Foundation, Washington, DC.
Pub. in Chemical Physics Letters 119, n1 p75-80, 23 Aug 85.

Keywords: *Bromine, *Dynamics, *Iodine halides, *Spin orbit interactions, Absorption, Reaction kinetics, Reprints, *Laser spectroscopy, *Iodine bromides.

A laser pulse-and-probe technique incorporating a tunable infrared color center laser is used to study the reactions and quenching of Br(doublet P(sub 1/2), doublet P(sub 3/2)) with IBr. A highly selective spin-orbit effect on chemical reactivity is observed. The ground-state reaction, Br(doublet P(sub 3/2)) + IBr yields Br₂ + I, $k = (4.6 \pm 0.6) \times 10^{-11}$ to the -11th power/cc molecule s proceeds at a rate $> \text{ or } = 40$ times faster than the rate of total Br (doublet P(sub 3/2)) quenching and reaction with IBr.

500,530
PB86-138450 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.

Morphology of Poly(ethylene terephthalate) Fibers as Studied by Multiple-Pulse (1)H NMR (Nuclear Magnetic Resonance).

Final rept.,
J. R. Havens, and D. L. VanderHart. 1985, 14p
Pub. in Macromolecules 18, n9 p1663-1676 1985.

Keywords: *Polyethylene terephthalate, *Nuclear magnetic resonance, Fibers, Molecular relaxation, Surfaces, Reprints, *Crystalline polymers.

Drawn poly(ethylene terephthalate) (PET) fibers annealed under various conditions are investigated by proton spin diffusion as detected through nuclear magnetic resonance. The primary objective is to study morphology on the 1-50-nm scale, the smaller dimensions of which have proved difficult to characterize for PET by conventional techniques. The spin diffusion experiment is comprised of three periods: generation of a magnetization gradient among different domains, relaxation of the gradient by diffusion for a variable time, and separate detection of the magnetization corresponding to each domain. The use of a multiple-pulse sequence permits spin diffusion to be confined to the second period, resulting in enhanced resolution among the domains. The procedure allows the magnetization decay observed during the detection period to be decomposed into three components, which are assigned to mobile noncrystalline, constrained noncrystalline, and crystalline domains. Rates of polarization redistribution among these three components are studied as a function of the diffusion time. Computer modeling is carried out in order to relate these measurements to the spatial arrangement and size of the three components. The results quantify the increase in crystallinity and in crystallite size upon annealing. Information pertaining to the structure of the noncrystalline region, the importance of noncrystalline chain orientation, and the relative surface areas of the crystallites is also presented.

500,531
PB86-138468 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Office of the Director.

Simple Accurate Absorption Model.

Final rept.,
K. F. J. Heinrich. 1985, 4p
Pub. in Proceedings of Annual Meeting of Electron Probe Microanalysis Society, Louisville, Kentucky, August 5-9, 1985, p79-82.

Keywords: *Absorption, *Mathematical models, *X ray analysis, Experimental design, Excitation.

A new model for the absorption of electron excited x-rays in the target, is proposed. This empirical model is simple and provides a good fit to existing experimental information. It will be particularly useful when elements of low (< 15) atomic numbers are determined.

500,532
PB86-138476 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Organic Analytical Research Div.

Quantitation of Individual Organic Compounds in Shale Oil.

Final rept.,
L. R. Hilpert, H. S. Hertz, W. E. May, S. N. Chesler, and S. A. Wise. 1979, 8p
Pub. in Proceedings of Oil Shale Symposium on Sampling, Analysis and Quality Assurance, Denver, Colorado, March 1979, p355-362 1980.

Keywords: *Shale oil, *Chemical analysis, *Environmental impacts, *Organic compounds, Gas chromatography, Mass spectroscopy, Phenols, Aromatic polycyclic hydrocarbons, Extraction, *Alternate fuels, *Toxic substances, High performance liquid chromatography, Standard reference materials.

A serious and largely unknown complication of developing alternate fuels such as shale oil is the potentially deleterious impact on the environment. Identification and quantitation of toxic organic compounds in the feedstock, process streams, and plant effluents will become increasingly important as mutagenicity testing on chromatographic fractions generated from various fuels and effluents expands. In preparation for certifying a Standard Reference Material for toxic constituents in alternate fuels, our laboratory has been investigating various techniques for quantitating individual organic compounds in shale oil. Emphasis has focused on acid-base extraction and high performance liquid chromatography as independent methods of shale oil fractionation. Gas chromatographic, gas chromatographic-mass spectro-metric, and high performance liquid chromatographic methods have been used to quantitate several phenols, N-heterocyclics, and polynuclear aromatic hydrocarbons in shale oil.

500,533
PB86-138484 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.

Charge Transfer, Vibrational Excitation, and Dissociative Adsorption in Molecule - Surface Collisions: Classical Trajectory Theory.

Final rept.,
S. Holloway, and J. W. Gadzuk. 1985, 13p
Pub. in Jnl. of Chemical Physics 82, n11 p5203-5215, 1 Jun 85.

Keywords: *Diatomic molecules, *Surface chemistry, Excitation, Potential energy, Adsorption, Molecular vibration, Dynamics, Reprints, *Atom diatom collisions.

The consequences of charge transfer processes occurring when a molecular beam of diatomic molecules is directed upon a solid surface are here considered. In analogy with resonance electron scattering from molecules or harpooning processes in atom-diatom collisions, the incident beam could either be scattered into a highly vibrationally excited molecular state, dissociatively scattered, or dissociatively adsorbed due to formation of temporary negative molecular ions which enable redistribution of the incident translation energy of the beam into intramolecular degrees of freedom. In the work, the exact classical trajectories for the diatomic molecule, including internal vibrational motion, are calculated for motion over model diabatic potential surfaces in which surface hopping due to charge transfer/harpooning is accounted for. Connections between classes of trajectories and topological features of the potential energy surfaces (PES) are illustrated. The model is used to study the average translational to vibrational energy transfer as a function of incident kinetic energy and of PES parameters. Branching ratios between scattered and dissociatively adsorbed molecules are obtained as a function of both incident translational and total energy and the role of the intermediate negative ion resonance in influencing the dynamics of molecular processes at surfaces is illustrated. Comparison with quantum mechanical theories is given in a subsequent paper.

500,534
PB86-138534 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Chemical Thermodynamics Div.

Kinetics of Peroxy Radical Reactions with Antioxidants.

Final rept.,
E. P. Hunter, and M. G. Simic. 1983, 6p
Pub. in Proceedings of Int. Conf. Superoxide and Superoxide Dismutase-Oxy Radicals Their Scavenger Syst. (3rd), v1 p32-37 1983.

Keywords: *Reaction kinetics, *Antioxidants, *Radiolysis, Activation energy, Viscosity, Phenols, *Peroxy radicals.

A variety of peroxy radicals were generated by pulse radiolysis in aqueous solutions and organic solvents and their rates with some phenolic antioxidants were measured. The rate constants depend on the nature of peroxy radicals, viscosity of the medium and temperature.

500,535
PB86-138567 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Inorganic Analytical Research Div.

Preliminary Studies of the Effects of Semiconductor Reagents on Polymers Containing Fluorine and of Trace Metallic Leachate from Molded Fluorocarbon Resin.

Final rept.,
J. F. Imbalzano, and J. R. Moody. 1985, 6p
Pub. in Jnl. of Environmental Sciences 28, p53-58 Jul/Aug 85.

Keywords: *Semiconductors, *Trace elements, *Metals, *Chemical analyses, *Polymers, Leaching, Diffusion, Exposures, Physical properties, Reprints, Vinylidene fluoride resins.

Traces of undesired materials in semiconductor devices are a serious processing deficiency and their elimination is widely sought. To this end, the effects of semiconductor reagents on discs molded from commercial materials of construction-perfluoroalkoxy (PFA) fluorocarbon resin and polyvinylidene fluoride (PVDF)-were assessed by measuring retained physical properties and by analytical microscopic inspection. At the National Bureau of Standards, Center for Analytical Chemistry, ultrapure nitric acid was stored, in a class 10 environment, in a container molded from PFA, and the level of leachable selected trace metallics was determined by graphite furnace atomic absorption spectrometry, flame emission spectrometry with repetitive optical scanning, and isotope dilution spark source mass spectrometry. The results from the exposure tests indicated that PVDF was significantly affected in the exposures; PFA was essentially unaffected. The amounts of leachable metallics from PFA were at or below low part-per-billion levels, since they were indistinguishable from those in the extractant blank.

500,536
PB86-138609 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Molecular Spectroscopy Div.

Reaction of F Atoms with the Methylhalides. Vibrational Spectra of CH₃X⁺ and of H₂CX...HF Trapped In Solid Argon.

Final rept.,
M. E. Jacox. 1985, 13p
Pub. in Jnl. of Chemical Physics 83, p3255-3267, 1 Oct 85.

Keywords: *Halides, *Vibration spectra, Chemical bonds, Photochemistry, Complex compounds, Infrared spectroscopy, Reprints, *Matrix isolation technique, *Fluorine atoms, *Chemical reaction mechanisms, Methane/chloro, Methane/bromo, Methane/iodo.

When the products of the reaction between F atoms formed in a microwave discharge and CH₃Cl, CH₃Br, or CH₃I were frozen in a large excess of argon at 14 K, the infrared spectra of the primary reaction products were obtained. Isotopic substitution experiments have provided evidence for two major reaction channels in each of these three reaction systems. Attack of the F atom at the halogen position results in the formation of the CH₃X⁺ addition product, which has a moderately strong X-F bond and is photochemically stable at wavelengths as short as 250 nm. F-atom reaction with a hydrogen atom of the methyl halide results in the stabilization of a weakly bound F-HCH₂X complex, intermediate to the formation of H₂CX + HF. For all of the species studied except CH₃Cl, the barrier to the decomposition of this complex is sufficiently great to require exposure of the solid deposit to visible light for the production of H₂CX and HF. The infrared spectra of the H₂CX-HF hydrogen-bonded complexes isolated in solid argon are discussed.

500,537
PB86-139789 Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Time and Frequency Div.

Field 7—CHEMISTRY

Group 7D—Physical Chemistry

Spectroscopy of Stored Atomic Ions.

Final rept.,
D. J. Wineland, W. M. Itano, J. C. Bergquist, J. J. Bollinger, and J. D. Prestage. 1984, 25p
Sponsored by Office of Naval Research, Arlington, VA., and Air Force Office of Scientific Research, Bolling AFB, DC.
Pub. in Proceedings of International Conference on Atomic Physics (9th), Seattle, Washington, July 23-27, 1984, p3-27.

Keywords: *Atomic spectra, Mass spectroscopy, Reviews, *Atomic ions, *Ion storage, Laser cooling, Laser spectroscopy.

In the paper, the authors briefly review measurements of atomic ion spectra made with the stored ion technique. Included are experiments on rf and optical spectra, mass spectra and laser cooling.

500,538

PB86-139839 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Viscosities and Glass Transition Pressures in the Methanol-Ethanol-Water System.

Final rept.,
I. Fujishiro, G. J. Piermarini, S. Block, and R. G. Munro. 1982, 3p
Pub. in Proceedings of 8th AIRAPT - 19th EHPRG Conference on High Pressure in Research and Industry, Uppsala, Sweden, August 17-27, 1981, v2 p608-611 1982.

Keywords: *Viscosity, *Transition points, *Methyl alcohol, *Ethyl alcohol, *Water, Mixtures, Pressure.

The pressure dependence of the viscosity and glass transition pressures for the binary methanol-water and ternary methanol-ethanol-water system have been measured at room temperature for several methanol-water compositions. A diamond-anvil falling-sphere viscometer, which uses the ruby fluorescence method of pressure measurement, was employed. Glass transition pressures were determined for the various mixtures by the ruby fluorescence line-broadening method. A new hydrostatic pressure transmitting medium was found having the composition 16 methanol: 3 ethanol: 1 water solution which extends the hydrostatic limit to 14.4 GPa at room temperature. A correlation between the pressure dependence of viscosity and the glass transition pressure is discussed for these solutions.

500,539

PB86-139896 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Inorganic Materials Div.

Spin Coupling through Oxygen. Influence of Structure and Solvent on doublet J((119)Sn,(117)Sn) in the (119)Sn NMR of Hexaorganodistannoxanes.

Final rept.,
T. P. Lockhart, W. F. Manders, and F. E. Brinckman. 1985, 6p
Sponsored by Office of Naval Research, Arlington, VA. Pub. in Jnl. of Organometallic Chemistry 286, p153-158 1985.

Keywords: *Oxygen, *Tin isotopes, *Molecular structure, Solvents, Molecular energy levels, Reprints, *Chemical shifts(Nuclear magnetic resonance), *Distannoxanes.

Sn,Sn spin coupling through oxygen, doublet J(119)Sn,(117)Sn, has been measured for seven hexaorganodistannoxanes (R₃Sn)₂O. The magnitude of the coupling constant depends strongly on the organic ligand, varying over the range 421 to 651 Hz in benzene solution. The substituent effect on doublet J is interpreted as arising from changes in the Sn-O-Sn bond angle, which should strongly influence the magnitude of the Fermi contact term contribution to the coupling constant. A pronounced solvent effect on doublet J(119Sn, 117Sn) was also observed; solvent studies with (n-Bu₃Sn)₂O indicate that the electron acceptor strength of the solvent determines the magnitude of the interaction. The utility of the coupling constant as a means of distinguishing between distannoxanes and related compounds is noted.

500,540

PB86-139904 Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.

Photodetachment Spectroscopy of -CH₂CN.

Final rept.,
K. R. Lykke, D. M. Neumark, V. J. Trapa, W. C. Lineberger, and T. Andersen. 1985, 4p
Grants NSF-PHY82-00805, NSF-CHE83-16628
Sponsored by National Science Foundation, Washington, DC.
Pub. in Proceedings of International Conference on Laser Spectroscopy (7th), Maui, Hawaii, Jun 24-28, 1985, p130-133.

Keywords: *Molecular structure, *Molecular energy levels, *Dynamics, Excitation, Line width, *Laser spectroscopy, *Methane/cyano, *Photodetachment.

High resolution photodetachment spectroscopy of -CH₂CN has been used to study the ionic ground state as well as an electronically excited dipole-bound state located in the vicinity of the threshold. The dynamical properties of the dipole-bound state have been investigated by means of line-width measurements. A surprising J dependence has been observed for the auto-detachment lifetimes.

500,541

PB86-139920 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Thermophysics Div.

Thermodynamic Properties of bcc Crystals at High Temperatures: The Transition Metals.

Final rept.,
R. A. MacDonald, and R. C. Shukla. 1985, 8p
Pub. in Physical Review B 32, n8 p4961-4968, 15 Oct 85.

Keywords: *Vanadium, *Niobium, *Tantalum, *Molybdenum, *Tungsten, *Thermodynamic properties, Perturbation theory, Body centered cubic lattices, Electronic specific heat, Transition metals, Reprints.

The second-neighbor central-force model of a bcc crystal, previously used in lowest-order anharmonic perturbation theory to calculate the thermodynamic properties of the alkali metals, is here applied to the transition metals V, Nb, Ta, Mo, and W. The limitations of the model are apparent in the thermal-expansion results, which fall away from the experimental trend above about 1800 K. The specific heat similarly fails to exhibit the sharp rise that is observed at higher temperatures. A static treatment of vacancies cannot account for the difference between theory and experiment. The electrons have been taken into account by using a model that specifically includes d-band effects in the electron ground-state energy. The results thus obtained for the bulk moduli are quite satisfactory. In the light of these results, the authors discuss the prerequisites for a better treatment of metals when the electrons play an important role in determining the thermodynamic properties.

500,542

PB86-139979 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Electrosystems Div.

Decomposition Products from Corona in SF₆/N₂ and SF₆/O₂ Mixtures.

Final rept.,
M. C. Siddagangappa, and R. J. Van Brunt. 1985, 4p
Sponsored by Department of Energy, Washington, DC. Div. of Electric Energy Systems.
Pub. in Proceedings of International Conference on Gas Discharges and Their Applications (8th), Oxford, England, September 16-20, 1985, p247-250.

Keywords: *Electric corona, *Decomposition reactions, Concentration(Composition), Nitrogen, Nitrogen oxides, Sulfur dioxide, Oxygen, Sulfur hexafluoride, Mixtures, Reaction kinetics.

Absolute concentrations of SOF₄, SOF₂, SO₂F₂, SO₂, NO, N₂O, and H₂O produced from continuous, dc, point-plane negative corona at a current of 40 A were measured in SF₆/N₂ and SF₆/O₂ mixtures containing trace amounts of H₂O and 1 to 95% N₂ or 1 to 10% O₂ for a total gas pressure of 200 kPa (about 2atm). The absolute and SF₆-normalized charge rates-of-production for these by-products have been determined as a function of N₂ or O₂ content. The results are interpreted in terms of a model for electric-discharge-induced decomposition of SF₆ discussed previously by Van Brunt. The presence of N₂ accelerates the rate of SF₆ decomposition by inhibiting the recombination of SF₆ dissociation products. At levels up to 10%, O₂ actually lowers the rates of oxyfluoride and SO₂ production due to its effect in reducing the mean energy of electrons in the discharge and thus the dissociation rate of SF₆.

500,543

PB86-140019 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Molecular Spectroscopy Div.

Reaction Products from a Discharge of N₂ and H₂S: The Microwave Spectrum of Two Conformers of Sulfur Diimide (HNSNH).

Final rept.,
R. D. Suenram, F. J. Lovas, and W. J. Stevens. 1985, 12p
Jnl. of Molecular Spectroscopy 112, p482-493 1985.

Keywords: *Molecular rotation, *Molecular structure, *Microwave spectroscopy, Dipole moments, Deuterium compounds, Reprints, *Molecular conformations, *Sulfur diimide.

The rotational spectra of two conformations of sulfur diimide (HNSNH) are reported. The HNSNH species are produced in a low-pressure microwave discharge of N₂ and H₂S. The microwave spectrum of the normal isotopic form, HNSNH, and deuterio form, DNSND, of the cis,trans and cis,cis forms have been observed. The electric dipole moment components of both forms have been determined. The molecular structures were determined from the experimental rotational constants and from geometry optimized ab initio calculations with 4-31G Gaussian basis sets and CEP-31G basis sets including polarization. The experimentally and theoretically derived molecular properties are found to be in good agreement.

500,544

PB86-140282 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Thermophysics Div.

Virial Coefficients of Ethylene.

Final rept.,
J. M. H. Levelt Sengers, and J. R. Hastings. 1981, 5p
Pub. in Proceedings of the Thermophysical Properties Symposium (8th), Thermophysical Properties of Fluids, Gaithersburg, Maryland, June 15-18, 1981, v1 p66-70.

Keywords: *Ethylene, *Virial coefficients, *Burnett method.

The authors report virial coefficients for ethylene, obtained in the vapor phase in the range 223-273 K by means of the Burnett method, at pressures from near saturation down to 0.23 MPa. The uncertainty of the pressure measurements is 5 parts in 10 to the 5th power; temperature was controlled and measured to better than 1 mK. Noxious volumes were absent. The data were tested for adsorption by coupling the isotherms isochorically; a small effect was found. Additional values of the second and third virial coefficient were derived from two sets of recent PVT data. Recent virial data from five sources, including the authors own, were correlated in the range 223 - 448 K by means of a simple empirical relationship. The data for the second virial from three of the sources generally agree to better than 0.5 cu cm/mol. Virials derived from speed-of-sound data are in excellent agreement with these data. There seems to be no need for further PVT data on low-density ethylene in the temperature range. Comparisons are also made of the predictions of two recent correlations of thermodynamic properties of ethylene. There is room for improvement, and suggestions are made as to how to achieve this.

500,545

PB86-140324 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.

What Can Polarized LEED Contribute to Surface Structure Determination.

Final rept.,
D. T. Pierce, R. J. Celotta, and G. C. Wang. 1984, 18p
Sponsored by Office of Naval Research, Arlington, VA. Pub. in Proceedings of the Conference on Determination of Surface Structure by LEED, Yorktown Heights, New York, June 19-20, 1980, p339-356 1984.

Keywords: *Surfaces, Tungsten, *Low energy electron diffraction, *Electron spin polarization, Polarized beams.

Polarized LEED (PLEED) has come of age in the sense data can now be measured along with spin averaged LEED data without requiring any extra time due to the availability of electron guns which produce intense beams of spin polarized electrons. The authors have measured a large set of data, including five non-specu-

lar beams and many specular beams, for the W(100) 1x1 unreconstructed surface. They also report PLEED measurements of the temperature and hydrogen induced phase changes in W(100). They hope availability of the data will stimulate more dynamical PLEED calculations, the comparison to which will definitively test the usefulness of PLEED in surface structure determination.

500,546

PB86-140340 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Fire Measurement and Research Div.
Thermal and Oxidative Degradation of Poly(Methyl Methacrylate): Weight Loss.
Final rept.,
T. Hirata, T. Kashiwagi, and J. E. Brown. 1985, 9p
Pub. in *Macromolecules* 18, n7 p1410-1418 1985.

Keywords: *Polymethyl methacrylate, *Thermal degradation, *Oxidation, Diffusion, Weight measurement, Comparison, Impurity, Samples, Reprints.

The effects of gas-phase oxygen on the weight loss of poly(methyl methacrylate) (PMMA) were studied by comparing weight loss behavior of PMMA degraded in nitrogen with that of PMMA degraded in air. Thermogravimetry (TG) and isothermal heating experiments were conducted to obtain kinetic constants for the degradation of PMMA. The results show that there are two distinct effects of oxygen on the weight loss of PMMA; one is an increase in PMMA stability at low temperatures and the other is destabilization of PMMA at high temperatures by enhanced random scission. There are two reaction stages for the weight loss from PMMA degraded in nitrogen and four reaction stages for PMMA degraded in air. These four reaction stages are, however, caused mainly by impurities in the sample. The effects of purification of the commercial PMMA on the weight loss are small for samples degraded in nitrogen, but they are significant for samples degraded in air.

500,547

PB86-140357 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Molecular Spectroscopy Div.
Spectroscopy and Photochemistry of Free Radicals Formed by the Reaction of F Atoms with Small Molecules.
Final rept.,
M. E. Jacox. 1985, 44p
Pub. in *Review of Chemical Intermediates* 6, p77-120 1985.

Keywords: *Spectrochemical analysis, *Photochemistry, *Free radicals, Chemical bonds, Infrared spectroscopy, Comparison, Reprints, *Matrix isolation techniques, *Fluoride atoms, *Chemical shifts(Nuclear magnetic resonance).

The techniques used for both gas phase and matrix isolation spectroscopic studies of the primary products of the reaction of F atoms with small molecules are surveyed. A review of the spectra of free radicals formed by F-atom reaction is presented, with emphasis on contributions of spectral studies to our understanding of the detailed reaction mechanism. When an F atom abstracts a H atom from a molecule trapped in solid argon, the resulting HF is hydrogen-bonded to the free radical product. Trapping of the R..HF species in solid argon somewhat strengthens the hydrogen bond compared to that typical of the gas-phase complex. An attempt is made to assess the extent of perturbation of the vibrations of the HF moiety by the argon matrix. Shifts in the vibrations of the free radical, R, as a result of the formation of R..HF are also considered.

500,548

PB86-142437 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymer Science and Standards Div.
Nonlinear Mechanical Behavior of Polymer Solutions at Various Concentrations.
Final rept.,
L. J. Zapas. 1982, 1p
Pub. in *Proceedings of IUPAC Macromol. Symposium* (28th), 1p 1982.

Keywords: *Mechanical properties, *Polymers, *Solutions, Concentration(Composition).

The reduction scheme proposed by Zapas and Phillips for concentrated polymer solutions, was derived for materials which obey certain conditions. In the paper it

is shown that these conditions were very strict, and more relaxed conditions give the same reduced properties even for a class of materials whose behavior can not be described with a single integral.

500,549

PB86-142445 Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Chemical Engineering Science Div.
Vapour-Liquid Equilibria Measurements for Carbon Dioxide with Normal and Isobutane from 250 to 280 K.
Final rept.,
L. A. Weber. 1985, 5p
Sponsored by Department of Energy, Washington, DC. Div. of Chemical Sciences.
Pub. in *Cryogenics* 25, p338-342 Jun 85.

Keywords: *Chemical equilibrium, *Carbon dioxide, Vapor phases, Liquid phases, Binary systems(Materials), Gibbs free energy, Reprints, *Isobutane.

Vapour-liquid equilibria measurements were made on binary mixtures of carbon dioxide with normal and isobutane at 250, 260, 270 and 280 K. Both liquid and vapour compositions were measured. The data correlated using the Peng-Robinson equation of state, and values are given for the activity coefficients and the excess Gibbs free energy, G(sup E). The heat of mixing is estimated from the temperature dependence of G(sup E).

500,550

PB86-142452 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Chemical Thermodynamics Div.
Thermodynamics of the Conversion of Aqueous Xylose to Xylulose.
Final rept.,
Y. B. Tewari, D. K. Steckler, and R. N. Goldberg. 1985, 5p
Pub. in *Biophysical Chemistry* 22, p181-185 1985.

Keywords: *Thermodynamics, *Chemical equilibrium, Heat measurement, Liquid phases, Enzymes, Gibbs free energy, Enthalpy, Isomers, Reprints, *Xylulose, High pressure liquid chromatography.

The thermodynamics of the conversion of aqueous xylose to xylulose has been investigated using high-pressure liquid chromatography (HPLC) and microcalorimetry. The reaction was carried out in aqueous phosphate buffer over the pH range 6.8-7.4 using solubilized glucose isomerase with MgSO₄ as a cofactor. The temperature range over which this reaction was investigated was 298.15-342.15 K. A combined analysis of both the HPLC and microcalorimetric data leads to the following results at 298.15 K for the conversion process. Comparisons are made with literature data.

500,551

PB86-142460 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Chemical Thermodynamics Div.
Investigation of the Equilibria between Aqueous Ribose, Ribulose, and Arabinose.
Final rept.,
Y. B. Tewari, and R. N. Goldberg. 1985, 8p
Pub. in *Biophysical Chemistry* 22, p197-204 1985.

Keywords: *Chemical equilibrium, *Thermodynamics, Heat measurement, Liquid phases, Enzymes, Enthalpy, Gibbs free energy, Isomers, Reprints, *Ribose, *Ribulose, *Arabinose, High pressure liquid chromatography.

The thermodynamics of the equilibria between aqueous ribose, ribulose, and arabinose were investigated using high-pressure liquid chromatography and microcalorimetry. The reactions were carried out in aqueous phosphate buffer over the pH range 6.8-7.4 and over the temperature range 313.15-343.75 K using solubilized glucose isomerase with either Mg(NO₃)₂ or MgSO₄ as cofactors. Information on rates of the reactions were also obtained.

500,552

PB86-142486 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.

Excimer Fluorescence Technique for Study of Polymer-Segment Mobility: Applications to Pyrene-Labelled Poly(methyl methacrylate) and Poly(methyl acrylate) in Solution.

Final rept.,
F. W. Wang, and R. E. Lowry. 1985, 7p
Pub. in *Polymer* 26, p1046-1052 Jul 85.

Keywords: *Polymethyl methacrylate, *Fluorescence, *Transport properties, Solutions, Pyrene, Viscosity, Reprints, *Poly(acrylic acid/(methyl-ester)), Excimers, Tracer techniques.

An excimer fluorescence technique for the study of polymer-segment mobility has been developed and applied to pyrene-labelled poly(methyl methacrylate) and poly(methyl acrylate) polymers in solution. The results of the study have been interpreted in terms of Kramers' theory for the crossing of a potential barrier by a particle embedded in a viscous medium. The results show that the internal viscosity has a solvent-independent part and lead to an estimate of the dimensionless internal viscosity parameter introduced by Cerf.

500,553

PB86-142635 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymer Science and Standards Div.
Critical Properties, Potential Force Constants, and Structure of Organic Molecules.
Final rept.,
I. C. Sanchez. 1985, 3p
Pub. in *American Institute of Chemical Engineers Jnl.* 31, n9 p1563-1565 Sep 85.

Keywords: *Critical points, *Molecular structure, *Alkanes, *Force, Temperature, Volume, Pressure, Van der Waals equation, Reprints, Carbon atoms, Oxygen atoms, Nitrogen atoms.

Recently, it was discovered that a certain combination of Lennard-Jones force constants varies linearly with the number of C, O, and N atoms in an organic molecule. The discovery implies that the product of the critical temperature T(sub c) and the 2/3 power of the critical volume V(sub c) and the product of the critical pressure P(sub c) and the 5/3 power of V(sub c) might also vary linearly with the number of C, O, and N atoms. The implication has been confirmed for a wide variety of organics.

500,554

PB86-142643 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.
Universal Coexistence Curve for Polymer Solutions.
Final rept.,
I. C. Sanchez. 1985, 4p
Pub. in *Applied Physics* 58, n8 p2871-2874, 15 Oct 85.

Keywords: *Polymers, *Solutions, *Solvents, *Mathematical models, Binary systems(Materials), Concentration(Composition), Reprints.

Coexistence curves for binary polymer/solvent solutions are asymmetric when volume fraction is used as the concentration variable. Coexistence curves for polystyrene/methylcyclohexane solutions can be symmetrized by a simple transformation of variables.

500,555

PB86-142684 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Fire Measurement and Research Div.
Spot Inception in a Methane/Air Diffusion Flame as Characterized by Detailed Species Profiles.
Final rept.,
K. C. Smyth, J. H. Miller, R. C. Dorfman, W. G. Mallard, and R. J. Santoro. 1985, 25p
Pub. in *Combustion and Flame* 62, p157-191 1985.

Keywords: *Soot, *Air pollution, *Flammability testing, *Combustion products, *Gas analysis, Concentration(Composition), Ionization, Fluorescence, Rayleigh scattering, Mass spectroscopy, Diffusion, Reprints, *Air pollution detection, Laser induced fluorescence, Laser induced ionization, Hydroxyl radicals.

Detailed species concentration profiles have been measured using optical and mass spectrometric methods in an atmospheric pressure methane/air diffusion flame burning on a Wolfhard-Parker slot burner. Rela-

Field 7—CHEMISTRY

Group 7D—Physical Chemistry

tive concentrations have been determined for OH by laser-induced fluorescence and, in addition, laser-induced production of C₂ has been monitored by fluorescence measurements. Broadband ultraviolet and visible fluorescence have been observed, and both are attributed to PAH, although other molecules may be responsible for these emissions at elevated temperatures. Small soot particles were detected by laser-induced ionization. Using a direct sampling mass spectrometer, absolute concentrations have been measured for methane, oxygen, nitrogen, carbon dioxide, water, hydrogen, acetylene, butadiene, and toluene. Profile measurements of several additional intermediate hydrocarbons have also been made, including methylacetylene (and/or allene), vinylacetylene, diacetylene, triacetylene, benzene, and naphthalene. These profiles are combined with velocity, temperature, and Rayleigh scattering measurements to characterize the region of chemical growth in a luminous diffusion flame.

500,556
PB86-142718 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Building Materials Div.
Effect of Water on Maleic Acid and Salicylic Acid Extractions.
Final rept.,
L. Struble. 1985, 6p
Grant NSF-CEE82-10791
Sponsored by National Science Foundation, Washington, DC.
Pub. in Cement and Concrete Research 15, p631-636 1985.

Keywords: *Maleic acid, *Salicylic acid, *Extractions, *Cement, *Water, Reprints.

Contamination of methanol by water was evidenced by the occurrence of ettringite in residues of cement extracted using a solution of maleic acid in methanol. Therefore, an analytical method was developed to determine water contents, based on the reaction of 2,2-dimethoxypropane with water, which forms acetone and methanol. Methanol analyzed by the method was found to contain as much as 2 percent H₂O. Thus it is necessary to use freshly dried methanol for extracting the silicates from cement or clinker. However, it was found that removal of all water causes the solution of maleic acid in methanol to gel when the cement or clinker is added, and the salicylic acid procedure is thus preferred because it does not form such a gel. It was shown that methanol containing levels of water as low as 0.5 percent will cause loss of water-soluble phases from cement or clinker.

500,557
PB86-142726 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymer Science and Standards Div.
Quasielastic Light Scattering from Dilute and Semidilute Polymer Solutions.
Final rept.,
D. W. Schaefer, and C. C. Han. 1985, 63p
Contract DE-AC04-76DP00789
See also DE82-016806. Sponsored by Department of Energy, Washington, DC.
Pub. in Dynamic Light Scattering, Chapter 5, p181-243 1985.

Keywords: *Light scattering, *Elastic scattering, *Polymers, *Dynamics, Spectroscopic analysis, *Photon correlations.

No abstract available.

500,558
PB86-142759 Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
State-Selective Photoionization and Photodissociation Spectroscopy of the H₂ Molecule from Excited States.
Final rept.,
H. Rottke, and K. Welge. 1985, 8p
Pub. in Jnl. de Physique 46, n1 pCL127-CL134 Jan 85.
Keywords: *Hydrogen, *Ionization, *Dissociation, *Photochemical reactions, Excitations, Molecular rotation, Molecular vibration, Reprints.

First experiments have been carried out on the two-step photoionization and photodissociation of the H₂ molecule from individual rotational-vibrational levels in the B(sup 1) sigma (+1) (sub u) state, employing tunable, pulsed, linearly polarized vuv and uv laser radi-

ation: High Rydberg states have been detected by field ionization, applied after the laser excitation pulse. Examples of ionization-dissociation spectra taken from v' = 0; J' = 0 and 1 levels in the B state are given. Also, some results obtained in dissociation region are reported.

500,559
PB86-142775 Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Chemical Engineering Science Div.
Non-Newtonian Flow of a Model Liquid between Concentric Cylinders.
Final rept.,
J. C. Rainwater, H. J. M. Hanley, T. Paszkiewicz, and Z. Petru. 1985, 9p
Sponsored by Department of Energy, Washington, DC. Office of Basic Energy Sciences.
Pub. in Jnl. of Chemical Physics 83, n1 p339-347, 1 Jul 85.

Keywords: *Non-newtonian fluids, *Mathematical models, *Liquids, Cylindrical bodies, Compressibility, Equations of motion, Pressure, Reprints, *Concentric cylinders, Computer applications, Numerical solution, Weissenberg effect.

Computer simulations of fluids out of equilibrium indicate that even the simplest fluid is in principle non-Newtonian. In particular, the simulations can provide explicitly the pressure tensor as a function of shear rate at a given temperature and density. In this paper the steady state flow of a model soft sphere liquid between rotating vertical concentric cylinders is discussed from a microscopic standpoint, given the coefficients that characterize the pressure tensor. The equations of motion are solved numerically. It is found that the normal pressure differences lead to an enhanced depression of the free surface at the inner cylinder, in contrast to a climbing (Weissenberg effect) which is usually regarded as the consequence of such differences. Reasons for the behavior observed for the soft sphere system are discussed. A consequence of the analysis is that a unique and self-consistent solution of the equations of motion is obtained only if the effects of finite compressibility are included.

500,560
PB86-142866 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Inorganic Analytical Research Div.
Resonance-ionization Mass Spectrometry of Carbon.
Final rept.,
L. J. Moore, J. D. Fassett, J. C. Travis, T. B. Lucatorto, and C. W. Clark. Sep 85, 5p
Sponsored by Department of Energy, Washington, DC. Office of Health and Environmental Research.
Pub. in Jnl. of the Optical Society of America B 2, n9 p1561-1565 Sep 85.

Keywords: *Carbon, *Chemical analysis, Mass spectroscopy, Graphite, Reprints, *Resonance ionization mass spectroscopy.

Resonance-ionization mass spectrometry (RIMS) for carbon has been demonstrated. A two-photon-resonant, three-photon ionization scheme provided large ionization signals from carbon atoms obtained by heating microgram samples of graphite. These results show that elemental carbon vapor can be detected at densities at least as low as 10 to the 7th power/cc. The feasibility of efficient resonance ionization is a first step to the development of a RIMS-analysis capability for elemental and isotopic carbon.

500,561
PB86-142924 Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Chemical Engineering Science Div.
Competitive Facilitated Transport through Liquid Membranes.
Final rept.,
K. Y. Niiya, and R. D. Noble. 1985, 16p
Pub. in Jnl. of Membrane Science 23, p183-198 1985.

Keywords: *Membranes, *Mathematical models, *Transport properties, *Gases, Chemical reactions, Diffusion, Mass transfer, Reprints.

A mathematical model is presented which solves the dimensionless, transient, non-linear partial differential equations governing the competitive facilitated transport of two gases through a liquid membrane. The model incorporates the mass transfer coefficients in the boundary conditions for the free gas concentra-

tions. Several studies were carried out. A comparison of this model with a steady-state 'equilibrium core' model was excellent. The idea of pumping one of the gases against its concentration gradient was shown to be theoretically possible.

500,562
PB86-143765 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymer Science and Standards Div.
Physical Modification of Properties of Semi-Crystalline Polymers.
Final rept.,
A. Peterlin. 1984, 53p
Pub. in Industrial Materials Science and Engineering, ch5 p145-197 1984.

Keywords: *Polymers, Physical properties, Revisions, Reprints, *Crystalline polymers.

No abstract available.

500,563
PB86-155561 PC A04/MF A01
National Bureau of Standards (NML), Gaithersburg, MD.
Summary of the Biological and Botanical Standards Issued by the National Bureau of Standards.
R. Mavrodineanu, and R. Alvarez. Oct 85, 75p NBS/SP-260/104, LCCCN-85-600605
See also PB84-165349. Also available from Supt. of Docs as SN003-003-02704-9. Library of Congress catalog card no. 85-600605.

Keywords: *Bioassay, *Materials, *Chemical analysis, *Botany, Environmental surveys, Clinical medicine, Physical properties, Chemical properties, Engineering standards, Research projects, *Standard reference materials, *Biological processes.

The publication is a summary of the biological and botanical Standard Reference Materials and Research Materials issued by the National Bureau of Standards. The material, composition, certification, use, and remarks concerning each of the ten materials described are presented in tabular form. Copies of the Certificates of Analysis for these materials are contained in the appendix for more detailed information.

500,564
PB86-155587 PC A07/MF A01
National Bureau of Standards (NML), Gaithersburg, MD. Office of Standard Reference Data.
Standard Reference Data Publications, 1964-1984.
J. C. Sauerwein, and G. R. Dalton. Dec 85, 147p NBS/SP-780
Supersedes PB82-134362. Also available from Supt. of Docs as SN003-003-02705-7. Library of Congress catalog card no. 85-600607.

Keywords: *Standards, Chemical properties, Physical properties, Bibliographies, Information systems, Indexes(Documentation), Computer programs, *Standard reference materials, Listings.

The National Bureau of Standards' Office of Standard Reference Data manages a network of data centers that prepare evaluated data bases of physical and chemical properties of substances. Data bases are available in printed form, on magnetic tapes and through on-line computer networks. This document provides a comprehensive list of the products available from the National Standard Reference Data System (NSRDS) for the years 1964-1984, including indexes qualified by author, material, and property terms. Ordering information and current prices can be found at the end of this document.

500,565
PB86-157336 PC A16/MF A01
National Bureau of Standards (NML), Gaithersburg, MD. Center for Chemical Physics.
Technical Activities 1985, Center for Chemical Physics.
P. Ausloos. Dec 85, 357p NBSIR-85/3257

Keywords: *Research projects, Surface chemistry, Reaction kinetics, Thermodynamics, Molecular spectroscopy, *Chemical physics.

The report summarizes research projects, measurement method development, testing and data evaluation activities carried out during Fiscal Year 1985 in the NBS Center for Chemical Physics. These activities fall in the areas of surface science, chemical kinetics,

chemical thermodynamics and molecular spectroscopy.

500,566

PC A04/MF A01

National Bureau of Standards, Gaithersburg, MD. Ceramics Div.

Comprehensive Method for the Determination of Aquatic Butyltin Species at Ultratrace Levels Using Simultaneous Hydridization/Extraction with GC-FPD.

Final rept.,

G. J. Olson, F. E. Brinckman, C. L. Matthias, and J.

M. Bellama. Dec 85, 51p NBSIR-85/3295

Prepared in cooperation with Maryland Univ., College Park. Dept. of Chemistry. Sponsored by David W. Taylor Naval Ship Research and Development Center, Annapolis, MD.

Keywords: *Water analysis, *Water pollution, *Biocides, Gas chromatography, Extraction, Chesapeake Bay, Concentration(Composition), Chemical analysis, Protective coatings, Toxicity, Metal containing organics compounds, Sampling, *Water pollution detection, *Tin/butyl, *Tin/butyl-methyl, *Tin/tributyl, *Tin/tetrabutyl, *Tin/dibutyl, Flame photometric detectors, Water pollution effects(Animals).

A method for the analysis of aquatic butyltin and mixed methylbutyltin species using simultaneous hydridization with sodium borohydride and extraction into dichloromethane is described. The detection limits are 7 ng Sn/L for tetrabutyltin, 7 ng Sn/L for tri-n-butyltin, 3 ng Sn/L for di-n-butyltin, and 16 ng Sn/L for mono-n-butyltin. The presence of tetrabutyltin in harbor waters is reported.

500,567

PC A06/MF A01

National Bureau of Standards, Gaithersburg, MD. Polymer Science and Standards Div.

Polymers: Technical Activities 1985.

Annual rept. 1 Oct 84-30 Sep 85,

L. E. Smith, and B. M. Fanconi. Nov 85, 104p

NBSIR-85/3190

Keywords: *Polymers, Reviews, Standards, Plastics, Performance evaluation, Blends, Mechanical properties, Composite materials, Molecular structure, Dental materials.

Technical Activities of the Polymers Division for FY 85 are reviewed. Included are descriptions of the 6 Tasks of the Division, project reports, publications, and other technical activities.

500,568

PC A99/MF E04

American Chemical Society, Washington, DC.

Atomic Energy Levels of the Iron-Period Elements: Potassium through Nickel,

J. Sugar, and C. Corliss. c1985, 680p ISBN-0-88318-480-X

Also pub. as Jnl. of Physical and Chemical Reference Data, v14 suppl2 1985. Library of Congress catalog card no. 85-72287. Prepared in cooperation with American Inst. of Physics, New York. Sponsored by National Bureau of Standards (NML), Gaithersburg, MD.

Keywords: *Atomic energy levels, *Potassium, *Calcium, *Scandium, *Titanium, *Vanadium, *Chromium, *Manganese, *Iron, *Cobalt, *Nickel, Ionization, Experimental design, Eigenvectors, *Isoelectronic sequence, Rydberg series.

Experimentally derived energy levels of the elements from potassium to nickel in all stages of ionization are critically compiled. The data for each level include its position in /cm (relative to the ground state), configuration, term designation, J-value, and, where available, the g-value and two leading percentages of the eigenvector composition in the most appropriate coupling scheme. For the He I and H I isoelectronic sequences, calculated level positions are given because they are considered more accurate than the measurements presently available. Ionization energies for each ion are derived either from Rydberg series, extrapolation, or calculation. Complete references are given for the compiled data.

500,569

PC A04/MF A01

National Bureau of Standards, Gaithersburg, MD. Ceramics Div.

Comprehensive Method for the Determination of Aquatic Butyltin Species at Ultratrace Levels Using Simultaneous Hydridization/Extraction with GC-FPD.

Final rept.,

G. J. Olson, F. E. Brinckman, C. L. Matthias, and J.

M. Bellama. Dec 85, 51p NBSIR-85/3295

Prepared in cooperation with Maryland Univ., College Park. Dept. of Chemistry. Sponsored by David W. Taylor Naval Ship Research and Development Center, Annapolis, MD.

Journal of Physical and Chemical Reference Data, Volume 14, Number 1, 1985.

Quarterly rept.

c1985, 400p

See also PB86-165461 through PB86-165511, and PB85-219830. Prepared in cooperation with American Inst. of Physics, New York. Sponsored by National Bureau of Standards, Gaithersburg, MD.

Available from American Chemical Society, 1155 16th St., NW, Washington, DC 20036.

Keywords: *Research projects, Molecular energy levels, Air, Thermal conductivity, Viscosity, Thermodynamic properties, Oxygen organic compounds, Specific heat, Enthalpy, Standards, Isomerization, Tables(Data), Electronic spectra, Density(Mass/volume), Binary systems(Materials), Oxygen, Nitrogen, Assessments, Critical point, Water, Heavy water, Deuterium compounds, Equations of state.

Contents:

Thermodynamic Properties of Key Organic Oxygen Compounds in the Carbon Range C1 to C4. Part 1. Properties of Condensed Phases;

Standard Chemical Thermodynamic Properties of Alkylbenzene Isomer Groups;

Assessment of Critical Parameter Values for H2O and D2O;

The Viscosity of Nitrogen, Oxygen, and Their Binary Mixtures in the Limit of Zero Density;

The Thermal Conductivity of Fluid Air;

The Electronic Spectrum and Energy Levels of the Deuterium Molecule;

Cumulative Listing of Reprints and Supplements.

500,570

PC A06/MF A01

National Bureau of Standards, Gaithersburg, MD. Polymer Science and Standards Div.

Polymers: Technical Activities 1985.

Annual rept. 1 Oct 84-30 Sep 85,

L. E. Smith, and B. M. Fanconi. Nov 85, 104p

NBSIR-85/3190

Keywords: *Polymers, Reviews, Standards, Plastics, Performance evaluation, Blends, Mechanical properties, Composite materials, Molecular structure, Dental materials.

Technical Activities of the Polymers Division for FY 85 are reviewed. Included are descriptions of the 6 Tasks of the Division, project reports, publications, and other technical activities.

500,571

PC A99/MF E04

American Chemical Society, Washington, DC.

Atomic Energy Levels of the Iron-Period Elements: Potassium through Nickel,

J. Sugar, and C. Corliss. c1985, 680p ISBN-0-88318-480-X

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Keywords: *Atomic energy levels, *Potassium, *Calcium, *Scandium, *Titanium, *Vanadium, *Chromium, *Manganese, *Iron, *Cobalt, *Nickel, Ionization, Experimental design, Eigenvectors, *Isoelectronic sequence, Rydberg series.

Experimentally derived energy levels of the elements from potassium to nickel in all stages of ionization are critically compiled. The data for each level include its position in /cm (relative to the ground state), configuration, term designation, J-value, and, where available, the g-value and two leading percentages of the eigenvector composition in the most appropriate coupling scheme. For the He I and H I isoelectronic sequences, calculated level positions are given because they are considered more accurate than the measurements presently available. Ionization energies for each ion are derived either from Rydberg series, extrapolation, or calculation. Complete references are given for the compiled data.

500,572

PC A04/MF A01

National Bureau of Standards, Gaithersburg, MD. Ceramics Div.

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Final rept.,

G. J. Olson, F. E. Brinckman, C. L. Matthias, and J.

M. Bellama. Dec 85, 51p NBSIR-85/3295

Prepared in cooperation with Maryland Univ., College Park. Dept. of Chemistry. Sponsored by David W. Taylor Naval Ship Research and Development Center, Annapolis, MD.

groups may be obtained by linear extrapolation. Equilibrium mole fractions within isomer groups have been calculated for the ideal gas state from 298.15 to 1000K. Values of specific heat, Enthalpy, entropy, and Gibbs energy are given for all species from C6H6 to C12H18 in joules for a standard state of pressure of 1 bar.

500,572

PC A04/MF A01

National Bureau of Standards (NEL), Gaithersburg, MD. Thermophysics Div.

Assessment of Critical Parameter Values for H2O and D2O,

J. M. H. Levelt Sengers, J. Straub, K. Watanabe, and P. G. Hill. c1985, 15p

Prepared in cooperation with Technische Univ., Munich (Germany, F.R.). Lehrstuhl A fuer Thermodynamik, Keio Univ., Yokohama (Japan). Dept. of Mechanical Engineering, and British Columbia Univ., Vancouver. Dept. of Mechanical Engineering.

Included in Jnl. of Physical and Chemical Reference Data, v14 n1 p193-207 1985. Available from American Chemical Society, 1155 16th St., NW, Washington, DC 20036.

Keywords: *Critical point, *Water, *Heavy water, *Steam, Assessments, Pressure, Temperature, Volume, Thermodynamic properties, Density(Mass/volume).

Recommendations for the most likely values of the critical parameters of light and heavy water as accepted by the International Association for the Properties of Steam are presented, together with an assessment of their reliability. Supporting material for these choices of values and the assessment of their reliability is provided. Temperature values are on the International Practical Temperature Scale of 1968 (ITS 1968) unless otherwise indicated.

500,573

PC A06/MF A01

National Bureau of Standards, Gaithersburg, MD. Polymer Science and Standards Div.

Polymers: Technical Activities 1985.

Annual rept. 1 Oct 84-30 Sep 85,

L. E. Smith, and B. M. Fanconi. Nov 85, 104p

NBSIR-85/3190

Keywords: *Polymers, Reviews, Standards, Plastics, Performance evaluation, Blends, Mechanical properties, Composite materials, Molecular structure, Dental materials.

Technical Activities of the Polymers Division for FY 85 are reviewed. Included are descriptions of the 6 Tasks of the Division, project reports, publications, and other technical activities.

The paper presents a concise and accurate representation of the viscosity of nitrogen, oxygen, and their binary mixtures at the limit of zero density and in the temperature range 110-2100K, which can be programmed easily on a computer. The correlation is founded upon the semiclassical kinetic theory of polyatomic gases and a body of critically evaluated experimental data. Use is also made of the principle of corresponding states to extend the correlation outside of the temperature range for which direct experimental results exist. The optimum correlation has an associated uncertainty of + or - 0.3% around room temperature, but it rises to a maximum of + or - 2% at either extreme of the temperature range. A secondary representation of the viscosity of the same gases, providing some saving in computational effort and a further extension of the temperature range at the expense of a small loss of accuracy, is also presented. The relationship of this second representation to similar correlations for other gases makes it attractive for some purposes.

500,574

PC A06/MF A01

National Bureau of Standards, Gaithersburg, MD. Polymer Science and Standards Div.

Polymers: Technical Activities 1985.

Annual rept. 1 Oct 84-30 Sep 85,

L. E. Smith, and B. M. Fanconi. Nov 85, 104p

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Keywords: *Polymers, Reviews, Standards, Plastics, Performance evaluation, Blends, Mechanical properties, Composite materials, Molecular structure, Dental materials.

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500,574

PC A06/MF A01

National Bureau of Standards, Gaithersburg, MD. Polymer Science and Standards Div.

Polymers: Technical Activities 1985.

Annual rept. 1 Oct 84-30 Sep 85,

L. E. Smith, and B. M. Fanconi. Nov 85, 104p

NBSIR-85/3190

Field 7—CHEMISTRY

Group 7D—Physical Chemistry

Keywords: *Thermal conductivity, *Air, Thermophysical properties, Thermodynamics, Equations of state, Density(Mass/volume), Fluids, Pressure, Temperature, Graphs(Charts).

Based on available experimental data, the thermal conductivity of fluid air has been critically evaluated. A new set of recommended values is presented covering a pressure range from 1 to 1000 bar and a temperature range from 70 to 1000K. Using the concept of residual thermal conductivity the recommended values are described by a 13-parameter equation of state in terms of temperature and density which may be applied up to a density of 900 kg/cu m. From comparisons of all data sources, the uncertainty of the recommended values was estimated to be below + or -4%. Additional experiments are needed, especially in the subcritical region of liquid air.

500,575

PB86-165511

Not available NTIS

Bell Labs., Murray Hill, NJ.

Electronic Spectrum and Energy Levels of the Deuterium Molecule,

R. S. Freund, and J. A. Schiavone. c1985, 149p

Prepared in cooperation with Argonne National Lab., IL. Sponsored by National Bureau of Standards, Gaithersburg, MD.

Included in Jnl. of Physical and Chemical Reference Data, v14 n1 p235-383 1985. Available from American Chemical Society, 1155 16th St., NW, Washington, DC 20036.

Keywords: *Molecular energy levels, *Electronic spectra, *Deuterium, Hydrogen isotopes, Tables(Data).

Beginning in the 1930s, G. H. Dieke and his students carried out an extensive program of measuring the optical spectrum of molecular hydrogen and its isotopes. Parts of the work were published but the project was interrupted by Dieke's death in 1965, with much of the latest and most accurate work unpublished. This paper gives the 27,488 lines of molecular deuterium, measured by Dieke, arranged the 8243 assigned lines into band systems, and derives rotational-vibrational energy levels for over 50 electronic states. It also derives energy levels from published vacuum ultraviolet spectra of D₂.

500,576

PB86-165529

Not available NTIS

American Chemical Society, Washington, DC.

Journal of Physical and Chemical Reference Data, Volume 14, Number 2, 1985.

Quarterly rept.

c1985, 241p

See also PB86-165537 through PB86-165552, and PB86-165453. Prepared in cooperation with American Inst. of Physics, New York. Sponsored by National Bureau of Standards, Gaithersburg, MD. Available from American Chemical Society, 1155 16th St., NW, Washington, DC 20036.

Keywords: *Research projects, Sulfur dioxide, Microwave spectroscopy, Astrophysics, Thermodynamics, Sodium chloride, Chemical equilibrium, Heat measurements, Viscosity, Polyethylene, Hamiltonian functions, Isotopes, Molecular vibration, Listings, Mark-Houwink-Sakurada equation.

Contents:

Microwave Spectra of Molecules of Astrophysical Interest. XXII. Sulfur Dioxide(SO₂);

Evaluation of the Thermodynamic Functions for Aqueous Sodium Chloride from Equilibrium and Calorimetric Measurements below 154C;

The Mark-Houwink-Sakurada Equation for the Viscosity of Linear Polyethylene;

Cumulative Listing of Reprints and Supplements.

500,577

PB86-165537

Not available NTIS

National Bureau of Standards (NML), Gaithersburg, MD. Molecular Spectroscopy Div.

Microwave Spectra of Molecules of Astrophysical Interest. 22. Sulfur Dioxide (SO₂),

F. J. Lovas. c1985, 94p

Included in Jnl. of Physical and Chemical Reference Data, v14 n2 p395-488 1985. Available from American Chemical Society, 1155 16th St., NW, Washington, DC 20036.

Keywords: *Microwave spectroscopy, *Sulfur dioxide, Astrophysics, Molecular vibration, Molecular energy levels, Molecular rotation, Sulfur 33, Sulfur 34, Sulfur 32.

The microwave spectrum of sulfur dioxide (SO₂) is critically reviewed and supplemented with spectral frequency calculations derived from rotational and centrifugal distortion terms in the molecular Hamiltonian. The primary objective of this review is to provide the microwave transition frequencies applicable to molecular radio astronomy for the ground vibrational state of the most abundant isotopic forms, i.e., the singly substituted atoms (33)S and (34)S.

500,578

PB86-165545

Not available NTIS

Dow Chemical of Canada Ltd., Sarnia (Ontario).

Evaluation of the Thermodynamic Functions for Aqueous Sodium Chloride from Equilibrium and Calorimetric Measurements below 154C,

E. C. W. Clarke, and D. N. Glew. c1985, 122p

Sponsored by National Bureau of Standards, Gaithersburg, MD.

Included in Jnl. of Physical and Chemical Reference Data, v14 n2 p489-610 1985. Available from American Chemical Society, 1155 16th St., NW, Washington, DC 20036.

Keywords: *Sodium chloride, *Chemical equilibrium, *Heat measurement, Solutions, Thermodynamic properties, Least square methods, Specific heat, Activity coefficients, Boiling point, Solubility, Tables(Data).

A new weighted least-squares method is described which is generally applicable for the nonsubjective evaluation of the best set of thermodynamic functions from a given data set of equilibrium (delta G) and calorimetric (delta H, C(sup p)) measurements. The method, applied to model a wide range of 2428 measurements for the water-sodium chloride system between -21 and 154C, accurately represents all measurements within experimental error. The resulting model is used to predict the thermodynamic functions and their standard errors for aqueous sodium chloride up to 110C. Tables are given for freezing point, solubility, boiling point, osmotic and activity coefficients, vapor pressure, apparent molal relative enthalpy, partial molal relative enthalpies, integral heat of solution, specific heat, apparent molal heat capacity, partial molal heat capacities, apparent molal relative heat capacity, partial molal relative heat capacities, standard thermodynamic functions, and their changes for dissolution.

500,579

PB86-165552

Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

Mark-Houwink-Sakurada Equation for the Viscosity of Linear Polyethylene,

H. L. Wagner. c1985, 7p

Included in Jnl. of Physical and Chemical Reference Data, v14 n2 p611-617 1985. Available from American Chemical Society, 1155 16th St., NW, Washington, DC 20036.

Keywords: *Polyethylene, *Viscosity, *Molecular weight, Decalin, Tetralin, Xylene, Chlorobenzenes, Solvents, Mark-Houwink-Sakurada equation, Benzene/trichloro, Naphthalene/chloro, Benzene/dichloro.

In this review, the parameters K and alpha found in the literature for the Mark-Houwink-Sakurada equation relating viscosity to molecular weight have been critically evaluated for linear polyethylene, and values have been recommended for six commonly used solvents. These are decalin, 1,2,4-trichlorobenzene, 1-chloronaphthalene, tetralin, o-dichlorobenzene, and p-xylene. In addition, the literature values of K for several different theta solvents are presented.

500,580

PB86-165560

Not available NTIS

American Chemical Society, Washington, DC.

Journal of Physical and Chemical Reference Data, Volume 14, Number 3, 1985.

Quarterly rept.

c1985, 225p

See also PB86-165578 through PB86-165636, and PB86-165644. Prepared in cooperation with American Inst. of Physics, New York. Sponsored by National Bureau of Standards, Gaithersburg, MD. Available from American Chemical Society, 1155 16th St., NW, Washington, DC 20036.

Keywords: *Research projects, Isotopes, Naphthalenes, Solubility, Mercury(Metals), Water, Electrolytes, Reviews, Phase transformations, Nitrogen, Alkenes, Thermodynamic properties, Phosphorus, Methane,

Heat of mixing, Liquids, Nucleation, Cations, Chemical bonds, Molecular energy levels, Phase equilibrium, PVT measurements, Listings.

Contents:

The Solubility of Mercury and Some Sparingly Soluble Mercury Salts in Water and Aqueous Electrolyte Solutions;

A Review and Evaluation of the Phase Equilibria, Liquid-Phase Heats of Mixing and Excess Volumes, and Gas-Phase PVT Measurements for Nitrogen + Methane;

The Homogeneous Nucleation Limits of Liquids; Binding Energies in Atomic Negative Ions:

II;

Energy Levels of Phosphorus, P I through P XV; Standard Chemical Thermodynamic Properties of Alkene Isomer Groups;

Standard Chemical Thermodynamic Properties of Alkyl naphthalene Isomer Groups;

Cumulative Listing of Reprints and Supplements.

500,581

PB86-165578

Not available NTIS

Emory Univ., Atlanta, GA. Dept. of Chemistry.

Solubility of Mercury and Some Sparingly Soluble Mercury Salts in Water and Aqueous Electrolyte Solutions,

H. L. Clever, S. A. Johnson, and M. E. Derrick.

c1985, 50p

Included in Jnl. of Physical and Chemical Reference Data, v14 n3 p631-680 1985. Available from American Chemical Society, 1155 16th St., NW, Washington, DC 20036.

Keywords: *Mercury(Metal), *Water, *Electrolytes, *Mercury inorganic compounds, Thermodynamics, Solutions, Inorganic salts, Solubility, Tables(Data).

The literature on the solubility of mercury and of the sparingly soluble salts of mercury(I) and mercury(II) in water and in aqueous electrolyte solutions has been reviewed. The solubility data have been compiled and evaluated. Recommended and tentative values of the solubilities are presented when warranted. Auxiliary thermodynamic data and crystallographic data useful in the interpretation of solubility data are given. An annotated bibliography on the solubility of some of the less common inorganic mercury compounds, with emphasis on the solubility literature published since 1950, is given.

500,582

PB86-165586

Not available NTIS

National Bureau of Standards (NEL), Boulder, CO. Center for Chemical Engineering.

Review and Evaluation of the Phase Equilibria, Liquid-Phase Heats of Mixing and Excess Volumes, and Gas-Phase PVT Measurements for Nitrogen + Methane,

A. J. Kidnay, R. C. Miller, E. D. Sloan, and M. J. Hiza. c1985, 14p

Included in Jnl. of Physical and Chemical Reference Data, v14 n3 p681-694 1985. Available from American Chemical Society, 1155 16th St., NW, Washington, DC 20036.

Keywords: *Nitrogen, *Methane, *Heat of mixing, *Binary systems(Materials), Reviews, Phase transformations, Gibbs free energy, *Phase equilibrium, *PVT measurements.

The available experimental data for vapor-liquid equilibria, heat of mixing, change in volume on mixing for liquid mixtures, and gas-phase PVT measurements for nitrogen + methane have been reviewed and where possible evaluated for consistency. The derived properties chosen for analysis and correlation were liquid mixture excess Gibbs free energies, and Henry's constants.

500,583

PB86-165594

Not available NTIS

Sibley School of Mechanical and Aerospace Engineering, Ithaca, NY.

Homogeneous Nucleation Limits of Liquids,

C. T. Avedisian. c1985, 35p

Sponsored by National Bureau of Standards, Gaithersburg, MD.

Included in Jnl. of Physical and Chemical Reference Data, v14 n3 p695-729 1985. Available from American Chemical Society, 1155 16th St., NW, Washington, DC 20036.

Keywords: *Liquids, *Nucleation, Graphs(Charts), Metastable states, Tables(Data).

The work provides a critical compilation of the homogeneous nucleation limits of liquids. Data for 90 pure substances and 28 mixtures have been compiled over a range of pressures, nucleation rates, and compositions. Detailed descriptions of the experimental methods used to obtain the included data are given to assess the accuracy of measured values. Criteria used to select the measurements included in the final listing are discussed.

500,584

PB86-165602 Not available NTIS
Joint Inst. for Lab. Astrophysics, Boulder, CO.

Binding Energies in Atomic Negative Ions: 2,
H. Hotop, and W. C. Lineberger. c1985, 20p
Included in Jnl. of Physical and Chemical Reference Data, v14 n3 p731-750 1985. Available from American Chemical Society, 1155 16th St., NW, Washington, DC 20036.

Keywords: *Cations, Reviews, Fine structures, Atomic energy levels, Excitation, *Electron affinity.

The article updates a ten-year-old review of this subject (J. Chem. Phys. Ref. Data 4, 539(1975)). A survey of the electron affinity determinations for the elements up to Z=85 is presented, and based upon these data, a set of recommended electron affinities is established. Recent calculations of atomic electron affinities and the major semiempirical methods are discussed and compared with experiment. The experimental methods which yield electron binding energy data are described and intercompared. Fine structure splittings of these ions and excited state term energies are given.

500,585

PB86-165610 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Center for Radiation Research.

Energy Levels of Phosphorus, P (I) through P (XV),
W. C. Martin, R. Zalubas, and A. Musgrove. c1985, 52p

Included in Jnl. of Physical and Chemical Reference Data, v14 n3 p751-802 1985. Available from American Chemical Society, 1155 16th St., NW, Washington, DC 20036.

Keywords: *Atomic energy levels, *Phosphorus, Ionization potentials, Optical spectra, Ions, Tables(Data), Isoelectronic sequence.

Energy level data are given for the atom and all positive ions of phosphorus (Z=15). 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 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.

500,586

PB86-165628 Not available NTIS
Massachusetts Inst. of Tech., Cambridge. Dept. of Chemistry.

Standard Chemical Thermodynamic Properties of Alkene Isomer Groups,
R. A. Alberty, and C. A. Gehrig. c1985, 18p
Sponsored by National Bureau of Standards, Gaithersburg, MD.

Included in Jnl. of Physical and Chemical Reference Data, v14 n3 p803-820 1985. Available from American Chemical Society, 1155 16th St., NW, Washington, DC 20036.

Keywords: *Alkenes, *Standards, *Thermodynamic properties, Enthalpy, Gibbs free energy, Entropy, Specific heat, Tables(Data).

The chemical thermodynamic properties of alkene isomer groups from C₄H₈ to C₆H₁₂ in the ideal gas phase have been calculated from 298.15 to 1000K from tables of Stull, Westrum, and Sinke. In the absence of literature data on all isomers of higher isomer groups, the properties of isomers of C₇H₁₄ to C₈H₁₆ have been estimated using Benson group values. Equilibrium mole fractions within isomer groups have been calculated for the ideal gas state from 298.15 to 1000K. For isomer group properties increments per carbon atom have been calculated to show the extent

to which thermodynamic properties of higher isomer groups may be obtained by linear extrapolation. Values of heat capacity, enthalpy, enthalpy of formation, and Gibbs energy of formation are given for all species from C₂H₄ to C₈H₁₆ in joules for a standard state of 1 bar.

500,587

PB86-165636 Not available NTIS
Massachusetts Inst. of Tech., Cambridge. Dept. of Chemistry.

Standard Chemical Thermodynamic Properties of Alkyl-naphthalene Isomer Groups,
R. A. Alberty, and T. M. Bloomstein. c1985, 17p
Sponsored by National Bureau of Standards, Gaithersburg, MD.

Included in Jnl. of Physical and Chemical Reference Data, v14 n3 p821-837 1985. Available from American Chemical Society, 1155 16th St., NW, Washington, DC 20036.

Keywords: *Naphthalene, *Thermodynamic properties, *Standards, Isomers, Specific heat, Entropy, Enthalpy, Gibbs free energy.

The chemical thermodynamic properties of alkyl-naphthalene isomer groups for C₁₀H₈ and C₁₁H₁₀ in the ideal gas phase have been calculated from 298.15 to 1000 K from tables of Stull, Westrum, and Sinke. In the absence of literature data on all isomers of higher groups, the properties of isomers of C₁₂H₁₂ to C₁₄H₁₆ have been calculated using Benson group values. A new Benson group value for the 1,8-dimethyl steric hindrance has been calculated from recent experimental data. The increments in isomer group properties per carbon atom 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 from 298.15 to 1000K. Values of heat capacity, entropy, enthalpy of formation, and Gibbs energy of formation are given for all species from C₁₀H₈ to C₁₄H₁₆ with energy units of joules for a standard state pressure of 1 bar.

500,588

PB86-165644 Not available NTIS
American Chemical Society, Washington, DC.

Journal of Physical and Chemical Reference Data, Volume 14, Number 4, 1985.

Quarterly rept.
c1985, 317p
See also PB86-165651 through PB86-165719, and PB86-165560. Prepared in cooperation with American Inst. of Physics, New York. Sponsored by National Bureau of Standards, Gaithersburg, MD.
Available from American Chemical Society, 1155 16th St., NW, Washington, DC 20036.

Keywords: *Research projects, Cyclohexanes, Density(Mass/volume), Temperature, Thermophysical properties, Carbon monoxide, Water, Refractivity, Wavelength, Viscosity, Thermal conductivity, Metals, Reaction kinetics, Free radicals, Tables(Data), Polystyrene, Thermodynamic properties, Cyclopentanes, Listings, Isomers, Hydrogen ions, Hydrogen atoms, Atom ion collisions, Superoxides, Mark Houwink Sakurada equation.

Contents:

Carbon Monoxide Thermophysical Properties from 68 to 100K at Pressures to 100 MPa;
Refractive Index of Water and Its Dependence on Wavelength, Temperature, and Density;
Viscosity and Thermal Conductivity of Dry Air in the Gaseous Phase;
Charge Transfer of Hydrogen Ions and Atoms in Metal Vapors;
Reactivity of HO₂/O₂(-1) Radicals in Aqueous Solution;
The Mark-Houwink-Sakurada Equation for the Viscosity of Atactic Polystyrene;
Standard Chemical Thermodynamic Properties of Alkylcyclopentane Isomer Groups, Alkylcyclohexane Isomer Groups, and Combined Isomer Groups;
Cumulative Listing of Reprints and Supplements.

500,589

PB86-165651 Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Chemical Engineering Science Div.

Carbon Monoxide Thermophysical Properties from 68 to 1000 K at Pressures to 100 MPa,
R. D. Goodwin. c1985, 84p

Included in Jnl. of Physical and Chemical Reference Data, v14 n4 p849-932 1985. Available from American Chemical Society, 1155 16th St., NW, Washington, DC 20036.

Keywords: *Carbon monoxide, *Thermophysical properties, Pressures, Equations of state, Temperature, Tables(Data).

An improved form of the nonanalytic equation of state is used to compute thermodynamic properties of carbon monoxide along isobars up to 100 MPa, at integral temperatures from coexistence to 1000K.

500,590

PB86-165669 Not available NTIS
Technische Univ., Munich (Germany, F.R.). Lehrstuhl A fuer Thermodynamik.

Refractive Index of Water and Its Dependence on Wavelength, Temperature, and Density,
I. Thormaehlen, J. Straub, and U. Grigull. c1985, 13p
Included in Jnl. of Physical and Chemical Reference Data, v14 n4 p933-945 1985. Available from American Chemical Society, 1155 16th St., NW, Washington, DC 20036.

Keywords: *Refractivity, *Water, *Steam, Equations of state, Graphs(Charts), Tables(Data), Least square methods.

A survey of the available experimental data and the existing equations for the refractive index of water is given. The dependence of the molar refraction on wavelength, temperature, and density is shown over an extended range. Based upon the electromagnetic theory of light an equation for the refractive index of water with wavelength, temperature, and density as independent variable is constructed. Its coefficients are directly deduced from all available experimental data by least-squares fit. Good agreement exists between the new relation, the available experimental data, and several existing equations.

500,591

PB86-165677 Not available NTIS
Keio Univ., Yokohama (Japan). Dept. of Mechanical Engineering.

Viscosity and Thermal Conductivity of Dry Air in the Gaseous Phase,

K. Kadoya, N. Matsunaga, and A. Nagashima. c1985, 24p
Sponsored by National Bureau of Standards, Gaithersburg, MD.
Included in Jnl. of Physical and Chemical Reference Data, v14 n4 p947-970 1985. Available from American Chemical Society, 1155 16th St., NW, Washington, DC 20036.

Keywords: *Viscosity, *Thermal conductivity, *Air, Transport properties, Temperature, Pressure, Graphs(Charts), Tables(Data), Dry methods.

In view of the importance of air in science and technology and the abundance of experimental data, the authors present in this report a consistent set of critically evaluated data and an up-to-date correlation of the thermal conductivity of air in the gaseous phase over a wide range of temperature and pressure. This is especially important for the viscosity, since the recent data show systematic differences compared with the old standard value used for many years. The present paper was written in order to document the critical evaluation of the latest data sets and to present a new set of correlations of the viscosity and thermal conductivity of air. The range covered is from 85 to 2000K for temperature and up to 100 MPa for pressure.

500,592

PB86-165685 Not available NTIS
Joint Inst. for Lab. Astrophysics, Boulder, CO.

Charge Transfer of Hydrogen Ions and Atoms in Metal Vapors,
T. J. Morgan, R. E. Olson, A. S. Schlachter, and J. W. Gallagher. c1985, 68p

Prepared in cooperation with Wesleyan Univ., Middletown, CT., Missouri Univ.-Rolla, and California Univ., Berkeley. Lawrence Berkeley Lab.
Included in Jnl. of Physical and Chemical Reference Data, v14 n4 p971-1040 1985. Available from American Chemical Society, 1155 16th St., NW, Washington, DC 20036.

Field 7—CHEMISTRY

Group 7D—Physical Chemistry

Keywords: *Metals, Chemical equilibrium, Graphs(Charts), Tables(Data), Excitation, *Hydrogen ions, *Hydrogen atoms, *Atom ion collisions, *Charge transfer cross sections, *Atom atom collisions, Collisional energy transfer.

Cross sections and equilibrium fractions for energetic H(+1), H(-1), and H(sup 0) in collisions with metal-vapor targets have been compiled and evaluated. Both experimental and theoretical results are reported. Sources of errors are discussed, and recommended values for the data are presented.

500,593

PB86-165693

Not available NTIS

Brookhaven National Lab., Upton, NY.

Reactivity of HO₂O₂(-1) Radicals in Aqueous Solution,

B. H. J. Bielski, D. E. Cabelli, R. L. Arudi, and A. B. Ross. c1985, 59p

Prepared in cooperation with Notre Dame Univ., IN. Radiation Chemistry Data Center. Sponsored by National Bureau of Standards, Gaithersburg, MD.

Included in Jnl. of Physical and Chemical Reference Data, v14 n4 p1041-1100 1985. Available from American Chemical Society, 1155 16th St., NW, Washington, DC 20036.

Keywords: *Free radicals, *Reaction kinetics, Solutions, Reviews, Tables(Data), Concentration(Composition), Absorption spectra, *Superoxides, *Perhydroxyl radical, *Oxygen ions, Chemical reaction mechanisms.

Kinetic data for the superoxide radical (HO₂ yields O₂(-1) + H(+1), pK=4.8) in aqueous solution have been critically assessed. Rate constants for reactions of O₂(-1) and HO₂ with more than 300 organic and inorganic ions, molecules and other transient species have been tabulated.

500,594

PB86-165701

Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

Mark-Houwink-Sakurada Equation for the Viscosity of Atactic Polystyrene,

H. L. Wagner. c1985, 6p

Included in Jnl. of Physical and Chemical Reference Data, v14 n4 p1101-1106 1985. Available from American Chemical Society, 1155 16th St., NW, Washington, DC 20036.

Keywords: *Polystyrene, *Viscosity, Solvents, Molecular weight, *Mark-Houwink-Sakurada equation.

In this review, the second in a series, the viscosity-molecular weight (Mark-Houwink-Sakurada) relationships have been critically evaluated for atactic polystyrene for a variety of solvents often used for viscosity measurements. These are benzene, toluene, 1,2,4-trichlorobenzene, tetrahydrofuran, o-dichlorobenzene, 2-butanone, and two theta solvents, cyclohexane and decalin. In addition, the Mark-Houwink-Sakurada parameters for several other solvents, not used as frequently, are provided.

500,595

PB86-165719

Not available NTIS

Massachusetts Inst. of Tech., Cambridge. Dept. of Chemistry.

Standard Chemical Thermodynamic Properties of Alkylcyclopentane Isomer Groups, Alkylcyclohexane Isomer Groups, and Combined Isomer Groups,

R. A. Alberty, and Y. S. Ha. c1985, 26p

Sponsored by National Bureau of Standards, Gaithersburg, MD.

Included in Jnl. of Physical and Chemical Reference Data, v14 n4 p1107-1132 1985. Available from American Chemical Society, 1155 16th St., NW, Washington, DC 20036.

Keywords: *Thermodynamic properties, *Cyclopentanes, *Cyclohexanes, *Standards, Specific heat, Gibbs free energy, Enthalpy, Entropy, Pressure, Tables(Data), *Isomers, Benson method.

The standard chemical thermodynamic properties of the alkylcyclopentane isomer groups have been calculated through C₉H₁₈ in the ideal gas phase from 298.15 to 1000K, and the properties of the alkylcyclohexane isomer groups have been calculated through C₁₀H₂₀. The properties of individual species for which literature data are not available have been estimated using the Benson method. The increments per carbon atom in the isomer group properties have been calculated to determine the extent to which extrapolations

may be made to higher carbon numbers. Since alkylcyclopentanes and alkylcyclohexanes of the same carbon number are isomers, the chemical thermodynamic properties of these combined isomer groups have also been calculated.

500,596

PB86-165776

PC A08/MF A01

National Bureau of Standards, Gaithersburg, MD.

Journal of Research of the National Bureau of Standards, Volume 90, Number 6, November-December 1985. Special Issue: Chemometrics Conference Proceedings.

Dec 85, 154p

See also PB86-165784 through PB86-165982, and PB86-137627. Also available from Supt. of Docs as SN703-027-00007-5.

Keywords: *Research projects, *Meetings, Chemical analysis, Calibrating, Reaction kinetics, Mathematical models, Spectroscopic analysis, Crystallography, Random walk, Chromatographic analysis, Polymers, Comparison, Experimental design, Electrochemistry, Pattern recognition, Kalman filtering, Procedures, Chemometrics.

Contents:

Topical issue:

Chemometrics;

Jack Youden;

The organizers' goals;

Agenda for chemometricians;

Adaptive Kalman filtering;

The limitations of models and measurements as revealed through chemometric

intercomparison;

Statistical properties of a procedure for analyzing pulse voltammetric data;

Fitting first order kinetic models quickly and easily;

The use of Kalman filtering and correlation techniques in analytical calibration procedures;

Intelligent instrumentation;

The regression analysis of collinear data;

Optimization;

Strategies for the reduction and interpretation of multicomponent spectral data;

Some new ideas in the analysis of screening designs;

Polymers and random walks-renormalization group description and comparison with experiment;

Fourier representations of Pdf's arising in crystallography;

Aggregated Markov processes and channel gating kinetics;

Automated pattern recognition;

Self-generating expert systems for the future;

Regression analysis of compartmental models;

Measurement and control of information content in electrochemical experiments;

Pattern recognition studies of complex chromatographic data sets.

500,597

PB86-165784

(Order as PB86-165776, PC A08/MF A01)

National Bureau of Standards, Gaithersburg, MD.

Topical Issue: Chemometrics,

H. J. Oser. Dec 85, 1p

Included in Jnl. of Research of the National Bureau of Standards, v90 n6 p391 Nov-Dec 85.

Keywords: *Meetings, Chemical analysis, *Chemometrics.

The issue of the NBS Journal of Research is devoted entirely to one topic: Chemometrics. A conference by that title held earlier this year at NBS brought together experts in analytical chemistry and applied mathematics, disciplines which are the constituents of this new field. This conference was probably the first one in the United States by that title. The roots of the interdisciplinary effort go back to the late Dr. William (Jack) Youden and the authors dedicate this issue to him. A brief description of Youden's career serves at the introduction to the collection of conference papers which the authors present in this volume of the Journal. The authors of this biographical sketch, Drs. Ku and DeVoe, worked very closely with Youden while he was at NBS. With the publication of the papers presented at this conference the authors hope to stimulate further work in the field of chemometrics. Special recognition goes to the organizers of the conference who also served as invited editors of this special issue of the NBS Journal of Research: Drs. Clifford H. Spie-

gelman of the Center for Applied Mathematics, Robert L. Watters of the Center for Analytical Chemistry, and Jerome Sacks from the University of Illinois.

500,598

PB86-165800

(Order as PB86-165776, PC A08/MF A01)

National Bureau of Standards, Gaithersburg, MD.

Organizers' Goals,

C. H. Spiegelman, R. L. Watters, and J. Sacks. Dec 85, 2p

Prepared in cooperation with Illinois Univ. at Urbana-Champaign.

Included in Jnl. of Research of the National Bureau of Standards, v90 n6 p395-396 Nov-Dec 85.

Keywords: *Research projects, *Management planning, *Chemometrics.

The wide range of disciplines represented by the participants and attendees of the Chemometrics Research Conference held at the Gaithersburg Holiday Inn on May 20-22, 1985, exemplifies the depth and diversity of the chemometrics community. The Conference was sponsored by several important professional societies whose members are involved in chemometric activity. As organizers, the authors had two main goals in mind when deciding on the form and substance of the Conference. The first was to provide a forum for reporting on some of the most recent and important research activities in diverse areas relating to chemometrics. The second and more important goal can only be achieved gradually. This was to increase the willingness of chemists, statisticians, and probabilists to meet as colleagues and to solve problems as a team. This will necessarily involve the exercise of communication skills as well as combining scientific skills.

500,599

PB86-165818

(Order as PB86-165776, PC A08/MF A01)

Wisconsin Univ.-Madison.

Agenda for Chemometricians,

W. G. Hunter. Dec 85, 6p

Sponsored by National Bureau of Standards, Gaithersburg, MD.

Included in Jnl. of Research of the National Bureau of Standards, v90 n6 p397-402 Nov-Dec 85.

Keywords: *Research projects, Chemical analysis, Statistical analysis, Management planning, Experimental design, *Chemometrics, Statisticians, Chemists.

No abstract available.

500,600

PB86-165834

(Order as PB86-165776, PC A08/MF A01)

National Bureau of Standards, Gaithersburg, MD.

Limitations of Models and Measurements as Revealed Through Chemometric Intercomparison,

L. A. Currie. 1 Jul 85, 14p

Included in Jnl. of Research of the National Bureau of Standards, v90 n6 p409-422 Nov-Dec 85.

Keywords: *Chemical analysis, Linear regression, Comparison, Mathematical models, Laboratories, Sampling, Measurement, Units of measurement, *Chemometrics, Intercomparison, Reference materials, Case studies.

Interlaboratory Comparisons using common (reference) materials of known composition are an established means for assessing overall measurement precision and accuracy. Intercomparisons based on common data sets are equally important and informative, when one is dealing with complex chemical patterns or spectra requiring significant numerical modeling and manipulation for component identification and quantification. Two case studies of 'Chemometric Intercomparison' using Simulation Test Data (STD) are presented, the one comprising STD vectors as applied to nuclear spectrometry, and the other, STD data matrices as applied to aerosol source apportionment. Generic information gained from these two exercises includes: (a) the requisites for a successful STD intercomparison (including the nature and preparation of the simulation test patterns); (b) surprising degrees of bias and imprecision associated with the data evaluation process, per se; (c) the need for increased attention to implicit assumptions and adequate statements of uncertainty; and (d) the importance of STD beyond the Intercomparison-i.e., their value as a chemometric

research tool. Open research questions developed from the STD exercises are highlighted, especially the opportunity to explore 'Scientific Intuition' which is essential for the solution of the underdetermined, multicollinear inverse problems that characterize modern Analytical Chemistry.

500,601
PB86-165842

(Order as PB86-165776, PC A08/MF A01)
Massachusetts Inst. of Tech., Cambridge.
Statistical Properties of a Procedure for Analyzing Pulse Voltammetric Data,
T. P. Lane, J. J. O'Dea, and J. Osteryoung. 24 Jun 85, 9p
Prepared in cooperation with State Univ. of New York at Buffalo. Sponsored by National Bureau of Standards, Gaithersburg, MD.
Included in Jnl. of Research of the National Bureau of Standards, v90 n6 p423-431 Nov-Dec 85.

Keywords: *Electrical measurements, *Mathematical models, Autocorrelation, Error analysis, Kinetics, Confidence limits, *Voltammetry, Maximum likelihood estimation, Procedures.

O'Dea et al. (1983, J. Phys. Chem. 97, 3911-3918) proposed an empirical procedure for obtaining estimates and confidence intervals for kinetic parameters in a model for pulse voltammetric data. Their goal was to find a procedure that would run in real time, not necessarily one that would have well-defined statistical properties. In this paper the authors investigate some of the statistical properties of their procedure. The authors show that their estimation method is equivalent to maximum likelihood estimation, and their confidence intervals, while related to likelihood ratio confidence regions, have a coverage probability that is not fixed and that is potentially quite large. The authors suggest modifications of their procedure that lead to more traditional confidence intervals. The authors examine the effect on their procedure of the presence of nuisance parameters. Finally, the authors discuss the possibility of serially correlated errors.

500,602
PB86-165859

(Order as PB86-165776, PC A08/MF A01)
Wisconsin Univ.-Madison.
Fitting First Order Kinetic Models Quickly and Easily,
D. M. Bates, and D. G. Watts. 24 Jun 85, 7p
Prepared in cooperation with Queen's Univ., Kingston (Ontario). Sponsored by National Bureau of Standards, Gaithersburg, MD.
Included in Jnl. of Research of the National Bureau of Standards, v90 n6 p433-439 Nov-Dec 85.

Keywords: *Reaction kinetics, *Mathematical models, Linear differential equations, Compartment analysis.

Kinetic models described by systems of linear differential equations can be fitted to data quickly and easily by taking advantage of the special properties of such systems. The estimation situation can be greatly improved when multiresponse data are available, since one can then automatically determine starting values and better discriminate between rival models.

500,603
PB86-165909

(Order as PB86-165776, PC A08/MF A01)
Emory Univ., Atlanta, GA.
Strategies for the Reduction and Interpretation of Multicomponent Spectral Data,
I. M. Warner, S. L. Neal, and T. M. Rossi. 1 Jul 85, 7p
Sponsored by National Bureau of Standards, Gaithersburg, MD.
Included in Jnl. of Research of the National Bureau of Standards, v90 n6 p487-493 Nov-Dec 85.

Keywords: *Fluorescence, *Spectrochemical analysis, Eigenvectors, Pattern recognition, Excitation, Molecular energy levels, Procedures.

Fluorescence data can be rapidly acquired in the form of an emission-excitation matrix (EEM) using a novel fluorometer called a video fluorometer (VF). An EEM array of 4096 data points composed of fluorescence intensity measured at 64 different emission wavelengths can be acquired in less than one second. The time-limiting factor in using this information for analytical measurement is the interpretation step. Consequently, sophisticated computer algorithms must be developed to aid in interpretation of such large data

sets. Recently, a new instrument has been described which rapidly acquires fluorescence detected circular dichroism (FDCD) data for chiral fluorophores as a function of multiple excitation and emission wavelengths. The FDCD matrix is similar in form to EEM data. However, since the FDCD matrix may have legitimate negative entries while the EEM is theoretically non-negative, different assumptions are required. This paper will describe the mathematical algorithms developed in this laboratory for the interpretation of the EEM in various forms. Particular emphasis will be placed on linear algebraic and two-dimensional Fourier Transform procedures.

500,604
PB86-165925

(Order as PB86-165776, PC A08/MF A01)
Chicago Univ., IL.
Polymers and Random Walks - Renormalization Group Description and Comparison with Experiment,
K. F. Freed. 1 Jul 85, 4p
Sponsored by National Bureau of Standards, Gaithersburg, MD.
Included in Jnl. of Research of the National Bureau of Standards, v90 n6 p503-506 Nov-Dec 85.

Keywords: *Polymers, *Random walk, Experimental design, Physical properties, Solutions, Molecular structure, Chemical bonds, Comparison, *Molecular configuration, Monomers.

Although real polymers involve the sequential addition of monomers having fixed bond lengths, fixed bond angles and some freedom of rotation about single bond, the properties of polymers over large length scales can be modeled by treating the polymer configuration as that of a random walk formed by the monomer units. Serious complications arise in the theoretical description of these polymers because of excluded volume constraints which prohibit different monomers from occupying the same position in space. This polymer excluded volume problem has been modeled in terms of a simple continuous random walk with short range repulsive interactions. The expansion of polymer properties in this repulsive interaction can readily be shown by dimensional analysis to involve an expansion in a large parameter, in the limit of long polymers. The renormalization group method is utilized as a systematic means for resuming this divergent perturbation expansion. The theory proceeds by analytically continued theory. The renormalization group approach is described from a heuristic physical standpoint and extensive comparisons are provided to show how it quantitatively reproduces vast amounts of dilute solution polymer properties with no adjustable parameters.

500,605
PB86-165941

(Order as PB86-165776, PC A08/MF A01)
California Univ., San Diego, La Jolla.
Aggregated Markov Processes and Channel Gating Kinetics,
D. R. Fredkin, and J. A. Rice. 1 Jul 85, 4p
Sponsored by National Bureau of Standards, Gaithersburg, MD.
Included in Jnl. of Research of the National Bureau of Standards, v90 n6 p517-520 Nov-Dec 85.

Keywords: *Markov processes, *Kinetics, Aggregates, Membranes, Ions, Mathematical models, Biochemistry, Proteins.

A finite state Markov process is aggregated into several groups. Rather than observing the underlying Markov process, one is only able to observe the aggregated process. What can be learned about the underlying process from the aggregated one. Such questions arise in the study of gating mechanisms in ion channels in muscle and nerve cell membranes. The authors discuss some recent results and their implications.

500,606
PB86-165958

(Order as PB86-165776, PC A08/MF A01)
Utah State Univ., Logan.
Automated Pattern Recognition: Self-Generating Expert Systems for the Future,
T. L. Isenhour. 1 Jul 85, 3p
Sponsored by National Bureau of Standards, Gaithersburg, MD.
Included in Jnl. of Research of the National Bureau of Standards, v90 n6 p521-523 Nov-Dec 85.

Keywords: *Pattern recognition, *Chemical analysis, Artificial intelligence, *Chemometrics, *Expert systems, Relational data bases, Robotics.

Chemometrics and pattern recognition had their start in chemistry in the late 1960's. The most recent review of the area by Micheal DeLaney listed 438 journal articles and books. The three most important areas of future development will be Expert Systems, Relational Data Bases, and Robotics. It should now be possible to combine existing robotics and artificial intelligence software to create a system which will generate its own expert systems using relational data bases. The data will be in the chemical domain and the system I describe the authors are calling the Analytical Director. The Analytical Director will be an artificial intelligence/robotic expert system for the analytical laboratory. The Analytical Director will develop, test, implement and interpret chemical analysis procedures. It will learn from its own experience, the experience of others and communicate what it has learned to others. The Analytical Director will be a self-generating Expert System. The author believes that such systems will, in the future, provide all the advantages of pattern recognition, expert systems and relational data bases in experimental settings. Problems will continue to be defined by human beings, but more and more, the laboratory will design, execute and evaluate its own experiments.

500,607

PB86-165974

(Order as PB86-165776, PC A08/MF A01)
Lawrence Livermore National Lab., CA.
Measurement and Control of Information Content In Electrochemical Experiments,
S. P. Perone, and C. L. Ham. 1 Jul 85, 11p
Sponsored by National Bureau of Standards, Gaithersburg, MD.
Included in Jnl. of Research of the National Bureau of Standards, v90 n6 p531-541 Nov-Dec 85.

Keywords: *Electrochemistry, *Chemical analysis.

One of the most important problems in chemical analysis is the interpretation of analytical data. The difficulty of this task has been further compounded by the data explosion. Chemical information relevant to the particular analysis problem is hidden within excessive amounts of data. This problem could be alleviated through knowledge and control of the information content of the data. Information theory provides a means for the definition, evaluation, and manipulation of quantitative information content measurements. This paper provides a general review of some of the basic concepts in information theory, including history, terminology, entropy, and other information content measures. The application of information theory to chemical problems requires some modifications. The analyst is usually only interested in a subset of the information (data) which has been collected. Also, this relevant chemical information is dependent upon not only the informational goals of the problem, but the completely specified procedure as well. This paper reviews chemical applications of information theory which have been reported in the literature including applications of information theory which have been reported in the literature including applications to qualitative analysis, quantitative analysis, structural analysis, and analytical techniques. Measures of information and information content and figures of merit for performance evaluations are discussed. The paper concludes with a detailed discussion of the application of information theory to electrochemical experiments and the empirical determination of the information content of electroanalytical data.

500,608

PB86-165982

(Order as PB86-165776, PC A08/MF A01)
Pennsylvania State Univ., University Park.
Pattern Recognition Studies of Complex Chromatographic Data Sets,
P. C. Jurs, B. K. Lavine, and T. R. Stouch. 24 Jun 85, 7p
Sponsored by National Bureau of Standards, Gaithersburg, MD.
Included in Jnl. of Research of the National Bureau of Standards, v90 n6 p543-549 Nov-Dec 85.

Keywords: *Pattern recognition, *Chromatographic analysis, *Spectrochemical analysis, Biochemistry, Classification, Assessments, Sampling, Biological processes.

Field 7—CHEMISTRY

Group 7D—Physical Chemistry

Chromatographic fingerprinting of complex biological samples is an active research area with a large and growing literature. Multivariate statistical and pattern recognition techniques can be effective methods for the analysis of such complex data. However, the classification of complex samples on the basis of their chromatographic profiles is complicated by two factors: (1) confounding of the desired group information by experimental variables or other systematic variations, and (2) random or chance classification effects with linear discriminants. The authors will treat several current projects involving these effects and methods for dealing with the effects. Complex chromatographic data sets often contain information dependent on experimental variables as well as information which differentiates between classes. Previously, Monte Carlo simulation studies were carried out to assess the probability of chance classification for nonparametric and parametric linear discriminants. The level of expected chance classification as a function of the number of observations, the dimensionality, and the class membership distributions were examined. These simulation studies established limits on the approaches that can be taken with real data sets so that chance classifications are improbable.

500,609
PB86-166808

(Order as PB86-166782, PC A04/MF A01)
National Bureau of Standards, Gaithersburg, MD.
Thermodynamics of Solution of SO₂(g) in Water and of Aqueous Sulfur Dioxide Solutions.
R. N. Goldberg, and V. B. Parker. 19 Jun 85, 18p
Included in Jnl. of Research of the National Bureau of Standards, v90 n5 p341-358 Sep-Oct 85.

Keywords: *Thermodynamics, *Sulfur dioxide, *Solutions, Water, Gibbs free energy, Specific heat, Enthalpy, Entropy, Chemical equilibrium, Heat measurement, Tables(Data), Oxidation.

A consistent set of thermochemical property values at 298.15K is given for the known constituents of aqueous sulfur dioxide. Also tabulated are values of the mean ionic activity coefficients, osmotic coefficients, partial pressure of SO₂(g), and the relative apparent molar enthalpy as a function of concentration of SO₂(aq) at 298.15K. The data analysis considered a wide variety of measurement techniques: calorimetric enthalpies of solution and reaction, heat capacities, equilibrium constants, solubilities, and vapor pressure measurement, both partial and total, over aqueous solutions of SO₂ for the temperature range 278 to 393K. All auxiliary data have been taken from the most recent set of CODATA values which were converted to a standard state pressure of one bar (0.1 MPa). Parameters are given which extend the predictions to temperatures up to 373K.

500,610
PB86-166832

(Order as PB86-166782, PC A04/MF A01)
National Bureau of Standards, Gaithersburg, MD.
Chemical Kinetics - Theory and Experiment.
Oct 85, 2p
Included in Jnl. of Research of the National Bureau of Standards, v90 n5 p389-390 Sep-Oct 85.

Keywords: *Reaction kinetics, *Meetings, Laboratories, Experimental design, Reviews, Chemical physics, Numerical solution.

The purpose of the conference was to bring together investigators from a broad range of institutions and backgrounds to review progress and problems in theoretical and experimental kinetics.

7E. Radio and Radiation Chemistry

500,611
PB85-202141

Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Pulse-Radiolysis and Gamma-Ray-Radiolysis of Cyclohexane - Ion Recombination Mechanisms.
Final rept.,
P. Ausloos, R. E. Rebert, F. P. Schwarz, and S. G. Lias. 1983, 17p
Pub. in Radiation Physics and Chemistry 21, n1-2 p27-43 1983.

Keywords: *Cyclohexane, *Radiolysis, Ions, Ethylene, Butadiene, Neutralization, Reprints, *Pulse radiolysis,

*Gamma ray radiolysis, Ion molecule interactions, Chemical reaction mechanisms, Ion fragmentation.

The products formed in the gamma-radiolysis and pulse-radiolysis of gaseous cyclohexane have been interpreted in terms of the ion fragmentation, ion-molecule reaction, and ion recombination mechanisms. It is shown that the fragmentation of the parent ion is partly quenched at a pressure of 55 torr. Ethylene and 1,3-butadiene are the major products resulting from electron neutralization of these ions. Fragmentation is strongly reduced when the neutralization process involves an atomic- or polyatomic-anion rather than an electron. For instance, addition of CCl₄ to cyclohexane results in a sharp drop of the yield of 1,3-butadiene, and a concurrent rise in the yield of 2-C₄H₈.

500,612
PB86-162211 PC A13/MF A01
National Bureau of Standards, Gaithersburg, MD.
Technical Activities 1985 - Center for Radiation Research.
C. E. Kuyatt. Oct 85, 288p NBSIR-85/3232
See also PB85-164952.

Keywords: *Research projects, *Radiation chemistry, *Nuclear physics, *Plasma radiation, Nuclear radiation, Laboratory equipment, Sources, Ionizing radiation, Atomizing.

The report summarizes research projects, measurement method development, calibration and testing, and data evaluation activities that were carried out during Fiscal Year 1985 in the NBS Center for Radiation Research. These activities fall in the areas of atomic and plasma radiation, radiation physics, radiometric physics, radiation sources and instrumentation, ionizing radiation, and nuclear physics.

8.

EARTH SCIENCES AND OCEANOGRAPHY

8D. Geochemistry

500,613
PB85-203438 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Nuclear and Chemical Dating Techniques: Interpreting the Environmental Record.
Final rept.,
L. A. Currie. 1982, 517p
Pub. in ACS (American Chemical Society) Symposium Series 176, p1-516 1982.

Keywords: *Geochemistry, *Archaeology, *Age estimation, *Radiocarbon dating, *Chemical analysis, Physicochemical properties, Meteorites, Trees(Plants), Ice formation, Sediments, Mass spectroscopy, Thermoluminescence, Isotope dating, Reprints, State of the art.

This volume is based on a symposium which took place at the March 1980 National ACS Meeting in Houston, Texas. The general objective of the Symposium was to review the latest developments and state-of-the-art of scientific (physicochemical) dating methods together with biogeochemical applications. In view of that objective the contents of this volume focus on advances in knowledge, testing of assumptions, and model validation which can be brought about through the use of complementary or multi-technique approaches--i.e., chemical vs nuclear chronometers, and dating with nuclides differing in decay characteristics and chemical behavior. Among the topics included are: advances in isotope mass spectrometry and low-level counting, resonance ion spectroscopy, direct atom counting with nuclear accelerators, amino acid racemization, thermoluminescence, and the extraction of isotopic and chemical records from meteorites, ice cores, sediment cores, and tree rings.

8E. Geodesy

500,614
PB85-229391 Not available NTIS
National Bureau of Standards (NML), Boulder, CO.
Quantum Physics Div.
JILA (Joint Institute for Laboratory Astrophysics) Portable Absolute Gravity Apparatus.
Final rept.,
J. E. Faller, Y. G. Guo, J. Gschwind, T. M. Niebauer, and R. L. Rinker. 1983, 12p
Sponsored by Air Force Geophysics Lab., Hanscom AFB, MA.
Pub. in Proceedings of the International Union of Geodesy and Geophysics General Assembly (18th), Hamburg, Germany, August 15-27, 1983, p87-97.

Keywords: *Gravimeters, *Gravity, Portable equipment, Accuracy, Laser interferometry.

At the Joint Institute for Laboratory Astrophysics, the authors have developed a new and highly portable absolute gravity apparatus based on the principles of free-fall laser interferometry. A primary concern over the past several years has been the detection, understanding, and elimination of systematic errors. In the Spring of 1982, the authors used the instrument to carry out a survey at twelve sites in the United States. The time required to carry out a measurement at each location was typically one day. Over the next several years, the intention is to see absolute gravity measurements become both usable and used in the field. To this end, and in the context of cooperative research programs with a number of scientific institutes throughout the world, the authors are building additional instruments (incorporating further refinements) which are to be used for geodetic, geophysical, geological, and tectonic studies. With these new instruments, the authors expect to improve (perhaps by a factor of two) on the 6-10 microgal accuracy of their present instrument. Today one can make absolute gravity measurements as accurately as -- possibly even more accurately than -- one can make relative measurements.

500,615
PB86-102951 Not available NTIS
National Bureau of Standards (NML), Boulder, CO.
Quantum Physics Div.
High Precision Gravity Measurements.
Final rept.,
I. Marson, and J. E. Faller. 1985, 15p
Pub. in Proceedings of the Conference on High Precision Geodetic Measurements, University of Bologna, Bologna, Italy, October 16-17, 1984, p314-328 1985.

Keywords: *Gravity, Geodesy, Measurement.

The measurement of the gravity acceleration is of interest in a broad area of physical sciences: metrology, geophysics and geodesy. High precision gravity data are required to study gravity variation with time, the motion of the Earth's core, and mass redistribution in the mantle and crust. In this paper, measurement techniques employed in high precision gravity devices are discussed.

500,616
PB86-123098 Not available NTIS
National Bureau of Standards (NML), Boulder, CO.
Time and Frequency Div.
Position Location Using Sequential GPS (Global Positioning System) Measurements.
Final rept.,
M. Weiss. 1982, 4p
Pub. in Proceedings of IEEE (Institute of Electrical and Electronics Engineers) Plans 82 Position Location and Navigation Symposium, Atlantic City, NJ., December 6-9, 1982, p275-278.

Keywords: Position(Location), Time measurement, Global positioning system.

The paper reports the development of a program to derive a first order correction to initial estimates of local coordinates and local clock bias from GPS time using a single channel GPS receiver of the C/A code. The program measures sequentially the local minus GPS time via four different satellites based on an initial estimate of local coordinates. Then using these measurements along with known locations of the satellites the first order corrections to the X, Y, and Z coordinates and the local time bias from GPS time are obtained.

8F. Geography

500,617
PB85-222859 CP T02
 National Bureau of Standards, Gaithersburg, MD. Inst. for Computer Sciences and Technology.
Countries, Dependencies, Areas of Special Sovereignty, and Their Principal Administrative Divisions (FIPS PUB 10-3).
 Data file.
 H. Tom, and J. Newton. 7 Jun 85, mag tape FIPS PUB 10-3, NBS/DF/MT-85/001
 Supersedes PB-267 936.
 Data file is available in the EBCDIC and ASCII character sets on 9-track one-half inch tape. Identify recording mode by specifying density and character set. Call NTIS Computer Products if you have questions.

Keywords: *Data file, *Geography, *Data processing, Standards, Magnetic tapes, Countries, Federal information processing standards, Data elements.

The file contains data from Table 1 of Federal Information Processing Standard Publication (FIPS PUB) 10-3 'Countries, Dependencies, Areas of Special Sovereignty, and Their Principal Administrative Divisions' including its change notices 1 and 2. The file includes the names and alphabetic two-character codes of each basic entity. In addition, it includes the name and four-character code of each principal division for those basic entities whose divisions are included in FIPS PUB 10-3. Records are sequenced in alphabetic order by basic entity. A typical entry consists of the country (basic entity) code and name and, if the basic entity is subdivided, the principal division codes and names. When printed out, each entry consists of the basic entity code and name on one line, followed by the principal division codes and names, one to each line. On lines with basic entity names, the last two characters of the code field are blank. Note that basic entity names are represented in UPPER CASE, while principal division names are in Mixed Case. Some principal divisions also have entries for conventional or former names. Conventional names are enclosed in (parentheses), while former names are enclosed in 'quotation marks'. Diacritics are not represented.

8G. Geology and Mineralogy

500,618
PB85-202638 Not available NTIS
 National Bureau of Standards, Gaithersburg, MD.
Loudounite, a New Zirconium Silicate Mineral from Virginia.
 Final rept.,
 D. E. Newbury, and P. J. Dunn. 1983, 4p
 Pub. in Canadian Mineralogist 21, n1 p37-40 Feb 83.

Keywords: *Silicate minerals, Zirconium compounds, Reprints, *Loudounite, Actinolite, Chlorite, Ancyrite.

Loudounite, $\text{NaCa}_5\text{Zr}_4\text{Si}_{16}\text{O}_{41}(\text{OH})_{11} \cdot 8\text{H}_2\text{O}$, is a new mineral from the Goose Creek Quarry, Loudoun County, Virginia, where it occurs as green to colorless spherules associated with actinolite, chlorite and ancyrite. The hardness is approximately 5 (Moh's); the density is 2.48(3) g/cc; and the streak is colorless. Loudounite is biaxial with wavy extinction, is length-slow, and has indices of refraction $\alpha = 1.536$ and $\gamma = 1.550$ (both + or - 0.004). Loudounite has also been found at the Fairfax Quarry, Centreville, Fairfax County, Virginia.

500,619
PB86-110160 Not available NTIS
 National Bureau of Standards (NML), Gaithersburg, MD. Office of Standard Reference Data.
Physical Properties Data of Rock Salt for Use in Designing Nuclear Waste Repositories.
 Final rept.,
 L. H. Gervantman. 1982, 7p
 Pub. in Proceedings of Symposium of AIME Annual Meeting on Process Mineralogy 2: Applications in Metallurgy, Ceramics, and Geology, Dallas, TX., February 14-18, 1982, p401-407.

Keywords: *Rock salt, Physical properties, Chemical properties, *Radioactive waste storage, Salt deposits.

A program for the compilation of evaluated physical and chemical numerical properties data is being pur-

sued at the National Bureau of Standards within the Office of Standard Reference Data. The intent is to assemble a reliable body of numerical properties data concerning candidate mineralogical materials in which high-level radioactive wastes are to be buried. The ready accessibility of the data to site designers and the credibility achieved through the evaluative process are designed to help assess and compare the feasibility of each candidate material for use as a disposal site. Both generic and site-specific data are to be assembled. To date, generic rock salt properties have been assembled and published by the NBS as NBS Monograph 167. Details of the effort to produce this book are discussed.

8I. Mining Engineering

500,620
PB85-178093 PC A10/MF A01
 Energy Analysts, Inc., Norman, OK.
Blowout Fire Simulation Tests. Final Report,
 D. B. Pfenning. Jan 85, 204p NBS/GCR-85/484

Keywords: *Blowouts, *Fire tests, Data, Oil wells, Gas wells, Fire fighting, Fire extinguishing agents, Water injection, Methane, Water spray.

The blowout of oil and gas wells during drilling, production, and workover presents a serious hazard to personnel, the environment, and equipment. The only practical method to control a well fire subsequent to a blowout is to shut in the hydrocarbon at the well. Although some individuals have effectively used water to mitigate well fire hazards, the quantitative effect of water sprayed into the fire zone is not known. To design effective oil and gas well blowout fire control systems, both the hazards associated with the fire and the efficiency of water to control fire hazards must be quantitatively understood. The Center for Fire Research (CFR) of the National Bureau of Standards has studied for the Department of the Interior the effectiveness of water spray to control and extinguish fires resulting from gas well blowouts. Laboratory scale tests have been performed by the CFR on 0.01-10 megawatt fires to study the effects of water injection on the combustion of high velocity methane jets. This report presents the results of two 100 megawatt and five 200 megawatt fire tests performed to measure the effects of water spray on fires from large velocity gas discharges characteristic of natural gas well blowouts.

500,621
PB85-232544 PC A10/MF A01
 National Bureau of Standards (NEL), Gaithersburg, MD. Center for Building Technology.
Application of Risk Analysis to Offshore Oil and Gas Operations - Proceedings of an International Workshop Held at Gaithersburg, Maryland on March 27 and 28, 1984.
 Final rept.,
 F. Y. Yokel, and E. Simiu. May 85, 213p NBS/SP-695
 Also available from Supt. of Docs as SN003-003-02650-6. Library of Congress catalog card no. 85-600525.

Keywords: *Meetings, *Offshore drilling, Gas production, Oil recovery, Specifications, Reliability, Offshore structures, Logistics support, Research management, Safety, Marine engineering, Operations, Petroleum industry, Regulations, Standards, *Risk analysis.

The proceedings of an International Workshop held at the National Bureau of Standards on March 27 and 28, 1984, are presented. The purpose of the workshop was to examine the application of risk analysis in offshore oil and gas operations. The proceedings include: an executive summary, an introduction, and summary reports and recommendations of four Working Groups: Standards, Codes, and Certification; Concept Evaluation and Design; Operation and Maintenance; and Logistics and Support. Also included are theme presentations on current practice in the United States, Great Britain, and Norway, and on current risk assessment methodologies.

8M. Soil Mechanics

500,622
PB85-184570 Not available NTIS
 National Bureau of Standards, Gaithersburg, MD.
Liquefaction Potential of Saturated Sand: The Stiffness Method.
 Final rept.,
 R. Dobry, D. J. Powell, F. Y. Yokel, and R. S. Ladd. 1980, 8p
 Sponsored by Turkish National Committee on Earthquake Engineering, Ankara., and Technical Univ. of Istanbul (Turkey).
 Pub. in Proceedings of World Conference on Earthquake Engineering (7th), Istanbul, Turkey, September 8-13, 1980, v3 p25-32.

Keywords: *Liquefaction, *Stiffness methods, *Sands, Sites, Evaluation, Saturated soils, Earthquakes, Design, Shear modulus, Stability, Earthquake engineering.

The paper proposes a new stiffness method for evaluating the liquefaction potential of horizontal saturated sand layers (level sites) during earthquakes. The method is based on field measurements of the shear modulus of the sand at small strains using geophysical techniques.

500,623
PB85-187854 Not available NTIS
 National Bureau of Standards, Gaithersburg, MD.
Liquefaction of Sands during Earthquakes - The Cyclic Strain Approach.
 Final rept.,
 F. Y. Yokel, R. Dobry, D. J. Powell, and R. S. Ladd. 1980, 10p
 Pub. in Proceedings of Int. Symposium on Soils Under Cyclic and Transient Loading 2, Swansea, England, January 7-11, 1980, p571-580.

Keywords: *Liquefaction, *Sands, *Earthquakes, Velocity, Secondary waves, Shear strain, Soil properties, Shear modulus, Tangent modulus, Evaluation, Predictions, Correlation, Earthquake engineering, Pore water pressure.

A method for evaluating the liquefaction potential of level sandy sites subjected to earthquake loads on the basis of anticipated cyclic shear strains is proposed. The data includes tests as well as test results. A method is proposed by which the maximum tangent shear modulus, which can be measured by shear wave propagation velocities, can be used to predict liquefaction potential.

500,624
PB85-208494 PC A05/MF A01
 National Bureau of Standards, Gaithersburg, MD.
Development of an NBS (National Bureau of Standards) Polymer Gage for Dynamic Soil Stress Measurement,
 R. M. Chung, A. J. Bur, and E. Reasner. Apr 85, 89p
 NBSIR-85/3135
 Sponsored by Air Force Armament Center, Elgin AFB, FL., and Air Force Engineering and Services Center, Tyndall AFB, FL. Engineering and Services Lab.

Keywords: *Measuring instruments, *Soils, *Stresses, Blast loads, Performance tests, Polymers, Protective coverings, Calibrating, Dynamic loads.

Polymer gages developed by the National Bureau of Standards (NBS) have been tested extensively in the NBS Geotechnical Engineering Laboratory to evaluate their capability and reliability for use in determining dynamic soil stresses generated by blast loadings. Penetration of soil grains into the gage surface was found to be the major concern and a major effort was undertaken to develop the most appropriate protective covering. Gages were dynamically loaded to develop their corresponding calibration curves.

500,625
PB86-114014 Not available NTIS
 National Bureau of Standards (NEL), Gaithersburg, MD. Structures Div.
Liquefaction Potential of Overconsolidated Sands in Areas with Moderate Seismicity.
 Final rept.,
 R. Dobry, F. Y. Yokel, and R. S. Ladd. 1981, 22p
 Pub. in Earthquakes and Earthquake Engineering 2, p643-664 1981.

Field 8—EARTH SCIENCES AND OCEANOGRAPHY

Group 8M—Soil Mechanics

Keywords: *Sands, *Earthquake resistant structures, *Liquefaction, Pore pressure, Shear strain, Shear strength, Saturated soils.

The liquefaction potential of a saturated sand depends on both the characteristics of the seismic shaking and of the soil. The paper reviews available evidence showing that overconsolidated sands have a larger resistance to liquefaction than normally consolidated sands, and it also presents new data from strain-controlled tests. Finally, the liquefaction potential of an overconsolidated sand site in Massachusetts, is discussed.

9.

ELECTRONICS AND ELECTRICAL ENGINEERING

9A. Components

500,626

PB85-182566 PC A02/MF A01
National Bureau of Standards (NEL), Gaithersburg, MD. Electrosystems Div.

Outline of CCVT (Coupling Capacitor Voltage Transformer) Calibration Procedure, EPRI-NBS (Electric Power Research Institute/National Bureau of Standards) Prototype System - Supplement to EPRI Report EL-690 (Field Calibration System for CCVTs, April 1978),
D. L. Hillhouse. Aug 84, 17p NBSIR-84/2987

Keywords: *Transformers, *Calibrating, *Coupling capacitor voltage transformers.

The report contains, in outline form, the step-by-step procedure for use of the EPRI-NBS Prototype Field Calibration System for Coupling Capacitor Voltage Transformers (CCVTs) in the calibration of CCVTs in the substation.

500,627

PB85-182582 PC A03/MF A01
National Bureau of Standards (NEL), Gaithersburg, MD. Electrosystems Div.

Development of Power System Measurements - Quarterly Report January 1, 1984 to March 31, 1984,

R. E. Hebner. Jul 84, 30p NBSIR-84/2898
Previously announced as DE84-017001. See also PB85-182590. Sponsored by Department of Energy, Washington, DC. Div. of Electric Energy Systems.

Keywords: *Electric fields, *Electrical measuring instruments, *Power transmission lines, Electric insulation, Dielectric breakdown, Insulating oil, Space charge, Sulfur hexafluoride, HVDC Systems, Ion counters.

The report documents the progress on three technical investigations sponsored by the Department of Energy and performed by the Electrosystems Division, the National Bureau of Standards. The work described covers the period from January 1, 1984 to March 31, 1984. The report emphasizes the performance of ion counters like those used to measure the ions near dc transmission lines, the production rates of oxyfluorides in SF₆ corona discharges, and the measurement of space charge associated with a pressboard interface in transformer oil.

500,628

PB85-182590 PC A03/MF A01
National Bureau of Standards (NEL), Gaithersburg, MD. Electrosystems Div.

Development of Power System Measurements - Quarterly Report April 1, 1984 to June 30, 1984,
R. E. Hebner. Mar 85, 40p NBSIR-85/3112
See also PB85-182582. Sponsored by Department of Energy, Washington, DC. Div. of Electric Energy Systems.

Keywords: *Electric fields, *Power transmission lines, Electrical measurement, Electrical insulation, Electric discharges, Sulfur hexafluoride, HVDC systems.

The report emphasizes the errors associated with measurements of dc electric fields, the properties of corona in compressed SF₆ gas, and the measurement of voltage pulses on nanosecond time scales.

500,629

PB85-182913 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.

Improved Concepts for Predicting the Electrical Behavior of Bipolar Structures in Silicon.

Final rept.,
H. S. Bennett. 1983, 8p
Pub. in IEEE (Institute of Electrical and Electronics Engineers) Transactions on Electron Devices 30, n8 p920-927 1983.

Keywords: *Field effect transistors, Silicon, Electrical properties, Carrier mobility, Predictions, Reprints.

Most bipolar device models contain empirical methods for computing the effective intrinsic carrier concentration, n_{sub} , mobility, and lifetime. These methods usually are based upon electrical measurements, assume that the majority hole (electron) mobility equals the minority hole (electron) mobility at high doping densities, use Boltzmann statistics, and assume that the carrier lifetime is much greater than the carrier transit time. More physically correct concepts are reported in this paper and are applied to bipolar transistors in silicon. These concepts use the perturbed densities of states and nonparabolic bands which arise from a quantum-mechanical description of bandgap narrowing to compute n_{sub} and the carrier mobility separately, use minority carrier lifetimes which agree much better with measured lifetimes in processed silicon, and use Fermi-Dirac statistics. When these concepts are incorporated into a device analysis code such as SEDAN and then used to compute the dc common-emitter gain of two npn transistors, the predicted gains agree very well with the measured gains. In addition, these concepts offer potential improvements in predicting the temperature dependence of the gain.

500,630

PB85-184752 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.

Reverse-Bias Second Breakdown of High Power Darlington Transistors.

Final rept.,
D. Y. Chen, F. C. Lee, D. L. Blackburn, and D. W. Berning. 1983, 8p
Prepared in cooperation with Virginia Polytechnic Inst. and State Univ., Blacksburg.
Pub. in IEEE (Institute of Electrical and Electronics Engineers) Transactions on Aerospace and Electronics Systems 19, n6 p840-847 Nov 83.

Keywords: *Transistors, Nondestructive tests, Reprints, *Second breakdown, *Darlington transistors, *Power transistors.

The reverse-bias second breakdown (RBSB) characteristics of high power Darlington transistors are discussed. The Darlington transistors investigated are rated at 400 V maximum voltage and 100 A maximum current. Devices both with and without speed-up diodes (connected between the bases of the input and output transistor) were studied. A nondestructive system for characterizing the RBSB behavior of these devices is described. The RBSB behavior was found to vary in an unpredictable manner with varying reverse base current magnitude. It was also found that the RBSB behavior of the Darlington transistors was a function of the forward base current magnitude. This is in marked contrast to what has been found for discrete devices. The presence of a speed-up diode also influenced the RBSB behavior of these devices.

500,631

PB85-187409 Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Fields Div.

Solid-State Reference Waveform Standard.

Final rept.,
R. A. Lawton, N. N. Nahman, and J. M. Bigelow. Sep 84, 5p
Pub. in IEEE (Institute of Electrical and Electronics Engineers) Transactions on Instrumentation and Measurement IM-33, n3 p201-205 Sep 84.

Keywords: *Waveforms, *Standards, Electric filters, Solid state devices, Reprints.

A solid-state reference waveform filter has been developed which uses the Maxwell-Wagner capacitor effect. This filter is realized in a stripline configuration with a lossy dielectric consisting of a thick (5 micrometers) layer of SiO₂ on Si. The equivalent circuit of this filter is equivalent to that for previously developed filters which used a lossy liquid dielectric. A preliminary design has been completed and a filter fabricated for which the design characteristic impedance, 38 ohms, and transition duration (rise time), 300 ps, agree with measured values to within 2 and 17 percent, respectively. The temperature dependence of the filter transition duration has been estimated from the temperature dependence of the filter conductance to be about 1 percent/C.

500,632

PB85-187805 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.

Behavior of the DC Impedance of an RF-Biased Resistive SQUID.

Final rept.,
D. Van Vechten, R. J. Soulen, and R. L. Peterson. 1980, 4p
Sponsored by Physikalisch-Technische Bundesanstalt, Berlin (Germany, F.R.), and European Physical Society, Geneva (Switzerland).
Pub. in Proceedings of IC SQUID Int. Conference on Superconducting Quantum Devices (2nd), Berlin, Germany, May 6-9, 1980, p186-189.

Keywords: *Electrical impedance, Josephson junctions, Nonlinear differential equations, Direct current, *SQUID devices, Superconducting weak links.

The authors have measured the dc impedance of an rf biased R-SQUID as a function of applied dc bias current, rf frequency and amplitude, and the critical current of the weak link. They conclude that the inclusion of an rf driving current, as required for parametric up-conversion influences, in an as yet incompletely modeled way, the dc impedance of an R-SQUID.

500,633

PB85-187839 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.

Semiconductor Device Simulation.

Final rept.,
C. L. Wilson, and J. L. Blue. 1981, 5p
Sponsored by Los Alamos Scientific Lab., NM.
Pub. in Proceedings of Elliptic Problem Solver Conference, Santa Fe, NM, June 30-July 2, 1980, p435-439 1981.

Keywords: *Semiconductor devices, *Mathematical models, Elliptic differential equations, Partial differential equations, Nonlinear differential equations, Metal oxide transistors, Solar cells, Simulation, Reprints, Bipolar transistors, Mesh generation.

The static simulation of semiconductor devices requires the solution of a system of three coupled nonlinear elliptic partial differential equations in two space dimensions. The solution of this system of equations is essential in simulation of bipolar and MOS transistors and more specialized devices such as large area photovoltaic cells and power transistors. This application presents two unusual problems which are a consequence of the exponential non-linearities which couple the system of equations. The exponential nature of the coupling imposes stringent accuracy requirements. These requirements are discussed in detail using a single elliptic equation in one space dimension. Extension of one-dimensional methods to two-dimensions requires some form of non-uniform, preferably adaptive, mesh generation so that reasonable accuracy can be obtained in the memory space of existing computers. The solution is also characterized by steep fronts whose location is strongly dependent on the value of the boundary condition. Small changes in these boundary values commonly result in large displacements of these fronts.

500,634
PB85-201523 Not available NTIS
 National Bureau of Standards, Gaithersburg, MD.
Microprocessor-Based Technique for Transducer Linearization.
 Final rept.,
 J. V. Moskaitis, and D. S. Blomquist. 1983, 2p
 Pub. in *Precis. Eng.* 5, n1 p5-8 Jan 83.

Keywords: *Transducers, *Calibrating, Microcomputers, Nonlinear algebraic equations, Cubic equations, Displacement, Detectors, Reprints, Sensors, Microprocessor, Computer software.

A linearization technique has been developed at the National Bureau of Standards (NBS) that is applicable to a wide range of transducers with calibration curves containing nonlinear regions. This technique was applied to a microcomputer-based, displacement sensor system that achieve accuracies of 1 part in 4096. By increasing the resolution of the ADC from 12 to 16 bits, a linearization of 1 part in 65,000 can be achieved.

500,635
PB85-202794 Not available NTIS
 National Bureau of Standards (NEL), Boulder, CO.
 Electromagnetic Technology Div.
Fast Detectors and Modulators.
 Final rept.,
 R. J. Phelan. 1984, 11p
 Pub. in *Semiconductors and Semimetals* 21, Part D p249-259 1984.

Keywords: Amorphous materials, Amorphous silicon, Optical modulators, Optical detectors, Picosecond pulses.

It is interesting to determine if a-Si:H can be used to create useful electro-optic devices with picosecond response speeds. Although one normally does not associate fast devices with low mobility materials, subnanosecond optical detectors and modulators have been made using hydrogenated amorphous silicon. Fast speeds are achieved by using very short lifetime materials or by making the structures sufficiently small that transit times are the limiting factor. A major factor favoring a-Si:H is the fact that it can be deposited on a wide variety of substrates allowing for the fabrication of structures that would otherwise be very difficult to construct.

500,636
PB85-205169 Not available NTIS
 National Bureau of Standards (NEL), Gaithersburg, MD. Electrosystems Div.
Operation of Ion Counters Near High Voltage DC Transmission Lines.
 Final rept.,
 R. H. McKnight, and P. M. Fulcomer. Jan 85, 3p
 Sponsored by Department of Energy, Washington, DC.
 Pub. in *Proceedings of Int. Symposium on High Voltage Engineering* (4th), Athens, Greece, September 5-9, 1983, Paper 64.03, 3p, Jan 85.

Keywords: *Power transmission lines, High voltage, Direct current, *Ion counters.

Measurements of electrical quantities such as electric field, vertical current density, and space charge density are necessary to characterize the electrical environment around high voltage dc transmission lines. Ion counters are used to measure space charge densities. A monopolar line has been used in the laboratory to study the effects of external electric fields on the operation of ion counters located above ground. Space charge densities were determined as functions of counter air flow, electrical potential, and inlet geometry. The effects of counter potential were not large until the potential was approximately equal to that of the space potential near the counter, when the indicated ion density dropped significantly. A dependence on flow rate was observed, which appears to be due to the large external electric fields existing at the inlet to the ion counter causing a loss of ions to the counter walls at lower flow rates.

500,637
PB85-206688 (Order as PB85-206324, PC A13/MF A01)
 Rome Air Development Center, Hanscom AFB, MA.
 Solid State Sciences Div.
Infrared Characterization of Defect Centers in Quartz.
 H. G. Lipson. Apr 85, 5p
 Included in *OM85: Basic Properties of Optical Materials. Summaries of Papers*, p145-149 Apr 85.

Keywords: *Quartz, *Crystal defects, *Crystal oscillators, *Infrared spectroscopy, Radiation effects, Frequency shift.

The radiation hardness and ageing properties of quartz oscillator devices depend strongly on the impurity and defect content of the synthetic quartz material. Low temperature infrared Fourier spectroscopy is a powerful tool for characterizing changes in quartz defect centers introduced by ionizing radiation and processing techniques such as electrodiffusion (sweeping). The technique of scanning large crystals normal to the growth of sweeping axis reported in this paper has revealed localized changes in defect center distribution produced by irradiation and the effect of impurity concentration on vacuum sweeping.

500,638
PB85-222073 Not available NTIS
 National Bureau of Standards (NML), Gaithersburg, MD. Radiometric Physics Div.
Recent Developments in the Technique for the Self-Calibration of Silicon Photodiodes.
 E. F. Zalewski. 1982, 10p
 Pub. in *Proceedings of Int. Symp. Technical Committee on Photon-Detectors of the Int. Measurement Confederation* (10th), Berlin, West Germany, September 20-22, 1982, p127-136.

Keywords: *Photodiodes, *Calibrating, Quantum efficiency, Silicon, *Self calibration.

Continuing research on the physics of silicon photodiodes has yielded a better understanding and several improvements in the technique for absolute response self-calibration. The author discusses the relationship between reverse bias measurements and the supralinearity effect, and shows how such measurements are a good test for diode quality. The author also discusses several new approaches to the oxide (front surface) bias measurements, and shows how the effects at the SiO₂-Si interface are related to the long-term stability of silicon photodiodes.

500,639
PB85-222339 Not available NTIS
 National Bureau of Standards (NML), Gaithersburg, MD. Radiometric Physics Div.
Quantum Yield of Silicon in the Ultraviolet.
 J. Geist. 1982, 5p
 Pub. in *Proceedings of Int. Symp. Technical Committee on Photon Detectors of the Int. Measurement Confederation* (10th), Berlin, West Germany, September 20-22, 1982, p49-53.

Keywords: *Photodiodes, *Silicon, *Quantum efficiency, Ultraviolet radiation, Self calibration.

Charge carriers produced in silicon by photons with energies above 3.4 eV can produce a second electron-hole pair by impact ionization, leading to a quantum yield that is greater than unity and that increases with photon energy. Accurate values of the quantum yield are required in order to extend the technique of silicon photodiode self-calibration into the ultraviolet spectral region. The author reports on recent experimental and theoretical studies that have yielded new and more accurate values for the quantum yield of silicon in the ultraviolet.

500,640
PB85-229839 Not available NTIS
 National Bureau of Standards (NEL), Gaithersburg, MD. Electrosystems Div.
EPRI-NBS (Electric Power Research Institute-National Bureau of Standards) Coupling Capacitor Voltage Transformer Calibration Systems.
 Final rept.,
 D. L. Hillhouse. 1985, 26p
 Sponsored by Electric Power Research Inst., Palo Alto, CA.
 Pub. in *Proceedings Workshop: Metering-type Coupling Capacitor Voltage Transformers (CCVTs)*, Gaithersburg, Maryland, June 2-3, 1983, p7-1--7-25 Apr 85.

Keywords: *Transformers, Calibrating, *Coupling capacitor voltage transformers, Metering.

The paper describes briefly a prototype system for field calibration of CCVTs developed by NBS in EPRI project RP-134-1, and in more detail, a simplified, less costly system developed later with partial support from the Pennsylvania Power and Light Co. The latter system was breadboarded as part of the above EPRI project. The prototype system contains five major dedicated components: (1) a current-comparator

bridge, (2) a modular capacitive transfer standard divider, (3) a compressed-gas standard capacitor, (4) a resonant power supply, and (5) a calibration truck. Its field accuracy is estimated to be 0.1% and 0.3 mrad, but it would be extremely expensive to reproduce. The simplified system contains only three major components: (1) the transfer standard divider above, (2) a voltage comparator, and (3) a combined standard-power transformer module. The latter two items represent much less cost and weight than items (2), (3) and (4) in the prototype system, which they replace.

500,641
PB85-229870 Not available NTIS
 National Bureau of Standards (NEL), Gaithersburg, MD. Electrosystems Div.
NBS (National Bureau of Standards) Experience, Field Calibration of Coupling Capacitor Voltage Transformers.
 Final rept.,
 D. L. Hillhouse. 1985, 15p
 Sponsored by Electric Power Research Inst., Palo Alto, CA.
 Pub. in *Proceedings Workshop: Metering-type Coupling Capacitor Voltage Transformers (CCVTs)*, Gaithersburg, Maryland, June 2-3, 1983, p1-1--1-14 Apr 85.

Keywords: *Transformers, Calibrating, Coupling capacitor voltage transformers, Metering.

Since its completion in 1976, the EPRI-NBS field calibration system for coupling capacitor voltage transformers (CCVTs) has been in NBS custody and has been used in field calibrations at six utilities. Measurements have been performed on 61 CCVTs, including 51 of metering class (12 of which were not using the X1X3 metering tap) and on nine metering VTs. The paper discusses the measurements at the six utilities, and summarizes all zero burden and connected burden results on metering windings. A large proportion of these CCVTs were found to be out of metering tolerance at both zero and connected burdens. However, the data base is not large enough to allow extension of these results to metering CCVTs in general.

500,642
PB86-102696 PC A04/MF A01
 National Bureau of Standards (NEL), Gaithersburg, MD. Center for Electronics and Electrical Engineering.
MOS1: A Program for Two-Dimensional Analysis of Si MOSFETs.
 Final rept.,
 C. L. Wilson, and J. L. Blue. Apr 85, 63p NBS/SP-400/77
 Also available from Supt. of Docs as SN003-003-02657-3. Library of Congress catalog card no. 85-600520. Color illustrations reproduced in black and white.

Keywords: *Metal oxide transistors, *Integrated circuits, Finite element analysis, Nonlinear differential equations, Partial differential equations, Computerized simulation, Electric current, Computer programs, *MOSFET, *Very large scale integration, MOS1 computer program, Fortran 77 programming language.

The MOS1 program is a portable FORTRAN 77 program suitable for analysis of currents and fields in VLSI devices. The program solves three coupled nonlinear elliptic partial differential semiconductor device equations in two dimensions. Historically, these equations have been solved using a special-purpose program and batch runs on a large, fast computer. The authors use a general-purpose program which runs on a large minicomputer or scientific workstation. This report discusses the physical formulation of the semiconductor equations and the methods used to select the solution strategy.

500,643
PB86-105715 PC A03/MF A01
 National Bureau of Standards (NEL), Gaithersburg, MD. Electrosystems Div.
High Voltage Divider and Resistor Calibrations.
 Final rept.,
 M. Misakian. Jul 85, 34p NBS/TN-1215
 Also available from Supt. of Docs as SN003-003-02672-7.

Keywords: *Voltage dividers, *Resistors, Electric reactors, High voltage, Direct current, Calibrating, Electrical properties, Standardization.

An NBS calibration service for determining the ratio of high voltage dc dividers and the resistance of high volt-

Field 9—ELECTRONICS AND ELECTRICAL ENGINEERING

Group 9A—Components

age resistors is described. Calibrations are performed with a Wheatstone bridge apparatus with a simple guard system. Sources of systematic error are identified and methods for characterizing the NBS standard high voltage resistors are discussed. Ratio and resistance values can be determined between the voltages of 10 kV and 150 kV with an uncertainty of less than + or -0.01%.

500,644
PB86-106739 PC A07/MF A01
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Applied Mathematics.
Generalizing the D-Algorithm,
J. S. Provan, and P. Domich. Sep 83, 129p NBSIR-83/2794

Keywords: *Integrated circuits, *Electrical faults, Reliability(Electronics), Tests, *Very large scale integration, *D algorithm, Fortran 77 programming language, Univac 1108 computers.

The authors consider the d-algorithm of J. P. Roth, which tests for specific faulty behavior in the integrated circuit. They develop a formal and general mathematical description of the algorithm, which allows a large degree of flexibility and extension in its implementation. They include a subsequent FORTRAN coding of such an extended d-algorithm, along with some sample testing.

500,645
PB86-112752 Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div.
Fabrication of a Miniaturized DCL (Direct-Coupled-Logic) OR Gate.
Final rept.,
R. H. Ono, J. A. Beall, and R. E. Harris. 1985, 4p
Pub. in IEEE (Institute of Electrical and Electronics Engineers) Transactions on Magnetics MAG-21, n2 p846-849 Mar 85.

Keywords: *Gates(Circuits), *Logic circuits, Josephson junctions, Superconductivity, Reprints, Electron beam lithography.

Using niobium edge junctions and electron beam lithography (EBL), the authors have made direct-coupled-logic (DCL) or gates with 1 micrometer minimum line widths. The gate cell, containing an isolator and a buffer section, fits into an area of approximately 25 by 30 square micrometers. The computer simulations show that these gates can have switching times of less than 10 ps. The authors have simulated the DCL circuit with several values of the most space-consuming element, an inductor. The paper describes the results of these simulations and presents a detailed description of the 7-level fabrication process. The mix of optical and electron-beam lithography used relies heavily on an inexpensive, yet powerful, circuit layout program.

500,646
PB86-112786 Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div.
Well Coupled, Low Noise, DC SQUIDS (Superconducting Quantum Interference Device).
Final rept.,
B. Muhlfeider, J. A. Beall, M. W. Cromar, R. H. Ono, and W. W. Johnson. 1985, 3p
Pub. in IEEE (Institute of Electrical and Electronics Engineers) Transactions on Magnetics MAG-21, n2 p427-429 Mar 85.

Keywords: Direct current, Reprints, *SQUID (Detectors).

The authors have designed, fabricated, and tested a Double Transformer (DT) coupled dc SQUID (Superconducting Quantum Interference Device) with low noise, an input inductance of 1 microH and a smooth input-output characteristic. A transmission line model is presented to explain a resonance in the input-output characteristic of early versions of this device. Guided by the results of numerical simulations a new version of this device has been built and tested. Experimental results are presented that show that the resonance can be moved to a higher voltage by reducing the area of the SQUID loop. The minimum detectable energy per unit bandwidth (MDE) referred to the SQUID loop, is 10h, where h is Planck's constant. Computer simulations indicate an MDE of 6h.

500,647
PB86-112810 Not available NTIS

National Bureau of Standards (NML), Boulder, CO. Time and Frequency Div.

Point Contact Diode at Laser Frequencies.
Final rept.,
K. M. Evenson, M. Inguscio, and D. A. Jennings. 1 Feb 85, 5p
Pub. in Jnl. of Applied Physics 57, n3 p956-960, 1 Feb 85.

Keywords: Tungsten, Nickel oxides, Reprints, *MIM diodes, *Point contact diodes.

Dramatic improvements in the stability of the metal-insulator-metal point contact diode has been achieved by the use of blunter whisker tips. The optimum values for tip radius and diode resistance were experimentally determined. Both sensitivity and high-speed response of W-NiO-Ni point contact diodes were investigated at different laser frequencies and mixing orders as a function of tip radius, resistance, and coupling. The tip radii were changed by more than an order of magnitude, and surprisingly, the sensitivity and the harmonic generation up to 88 THz were not significantly affected. A conical antenna was found to be superior to the conventional longwire antenna at wavelengths shorter than 10 micrometers. Responsivity measurements as a function of the diode resistance showed evidence for two different physical mechanisms responsible for the operation of the diode.

500,648
PB86-119278 Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Fields Div.
Chaos and Thermal Noise in the rf-Biased Josephson Junction.
Final rept.,
R. L. Kautz. 1985, 17p
Contract N00014-84-F-0038
Sponsored by Office of Naval Research, Arlington, VA.
Pub. in Jnl. of Applied Physics 58, n1 p424-440, 1 Jul 85.

Keywords: *Josephson junctions, Superconductivity, Reprints, Johnson noise, Chaos.

The effect of thermal noise on chaotic behavior in the rf-biased Josephson junction is studied through digital simulations. In instances for which chaotic behavior occurs in the noise-free system, it is found that the dynamics of the system are almost unchanged by the addition of thermal noise unless the level of thermal noise exceeds that of the chaotic state. In instances for which the only stable states of the noise-free system are periodic solutions, small amounts of thermal noise can induce the junction to hop between two different dynamical states, producing a low-frequency noise level much higher than that of the thermal noise. Such noise-induced hopping can occur either between two periodic solutions or between a periodic solution and a metastable chaotic solution. When a metastable chaotic state is involved, temperatures somewhat higher than those which produce hopping can destabilize the periodic solution to the point where the system spends virtually all of its time in the metastable chaotic state, creating noise-induced chaos. The similarities between chaotic behavior at zero temperature and noise-induced chaos are sufficiently strong that it may be difficult to distinguish the two cases experimentally.

500,649
PB86-119310 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Integrated-Circuit Metrology.
Final rept.,
W. M. Bullis. 1981, 3p
Pub. in EDN 26, n20 p120-122, 127, 14 Oct 81.

Keywords: *Integrated circuits, *Metrology, Silicon, Reprints, Semiconductors.

Projected trends in integrated circuit metrology during the next quarter century are discussed. The picture that emerges for the IC factory of 2006 is one of extensive computer control of both fabrication and characterization based on more complete understanding of the materials and processes employed. The metrological advances which will occur in the next quarter century may be expected both to enhance our fundamental understanding of the solid state and to provide the means for reliable and economical manufacture of more complex and more powerful integrated circuits.

500,650
PB86-123114 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiometric Physics Div.

Silicon Photodiode Self-Calibration as a Basis for Radiometry in the Infrared.

Final rept.,
E. Zalewski, and M. Tufino. 1981, 5p
Pub. in Proceedings of the Society of Photo-Optical Instrumentation Engineers-International Society of Optical Engineers 308, p2-6 1981.

Keywords: *Photodiodes, *Radiometry, *Calibrating, Infrared radiation, Silicon, *Self calibration.

The recently developed, simple and highly accurate technique for self-calibration of the absolute response of a silicon photodiode is described. The silicon photodiode self-calibration (SPSC) technique is independent of both electrical substitution radiometers (ESR's) and blackbodies - the traditional standards of absolute radiometry. Using the SPSC technique one can obtain high accuracy over a limited wavelength range with a very small investment of time and money. This means that the SPSC technique can be conveniently used to calibrate an ESR, thus avoiding the long and tedious characterization measurements required to evaluate the radiant to electrical power calibration factor of an ESR.

500,651
PB86-128790 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Semiconductor Materials and Processes Div.
Leak Testing of Hermetically Sealed Electronic Components.
Final rept.,
S. Ruthberg. 1982, 6p
Pub. in Proceedings of American Society for Nondestructive Testing Spring Conference, Boston, MA., March 22-25, 1982, and Fall Conference, Pittsburgh, PA., October 4-7, 1982, p431-436.

Keywords: *Electronic packaging, *Leakage(Electrical), Tests, Hermetic seals, Electric devices.

In the electronics industry the requirements are for leak testing large numbers of relatively small sealed packages to very fine leak rates. A wide variety of package materials are used; internal volumes range from less than 0.001 cubic cm. to greater than 10 cubic cm.; and the leak size reject level may be less than 1 x 10 to the minus 9 power Pa cubic m/s. No single test can cover the leak size range. Present preferred methods such as the radioisotope, helium leak detector, and others are assessed as to range, precision, efficiency, and usefulness as based upon fluid transport mechanisms and experimental data.

500,652
PB86-132610 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Semiconductor Devices and Circuits Div.
Turn-Off Failure of Power MOSFETS.
Final rept.,
D. L. Blackburn. 1985, 7p
Pub. in Proceedings of Annual IEEE (Institute of Electrical and Electronics Engineers) Power Electronics Specialists Conference (16th), Toulouse, France, June 24-28, 1985, p429-435.

Keywords: *Field effect transistors, Reliability(Electronics), Failure, *MOSFET, Bipolar transistors, Second breakdown.

Experimental results of the failure of power MOSFETs during inductive turn-off are discussed. The electrical characteristics of these devices during failure are shown to be identical to those of a bipolar transistor undergoing second breakdown. Other comparisons of the power MOSFET failure and bipolar second breakdown are made. A nondestructive measurement system is used which allows repeated measurements of the failure characteristics as a function of various parameters to be made on a single device.

500,653
PB86-133444 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Semiconductor Devices and Circuits Div.
Sensitivity Analysis of SPICE Parameters Using an Eleven-Stage Ring Oscillator.
Final rept.,
J. M. Cassard. 1984, 6p
Pub. in IEEE (Institute of Electrical and Electronics Engineers) Jnl. of Solid State Circuits SC-19, n1 p130-135, 1 Feb 84.

Keywords: *Circuits, *Simulators, Wafers, Simulation, Dynamic response, Sensitivity, CMOS, Chips(Electronics).

The paper presents examples of how well model parameters extracted from a test chip can predict the ac response of a dynamic circuit element on the same wafer. Simulation results show which model parameters are critical to performance. A comparison between measurement and simulation results is given and the importance of intrachip and intra-wafer parameter variations is discussed. For the samples tested, the polysilicon gate linewidth variation was determined to be the primary cause of the ring oscillator frequency variation.

500,654
PB86-134962

(Order as PB86-134871, PC A09/MF A01)
National Bureau of Standards (NEL), Gaithersburg, MD. Electrosystems Div.

Approach to ATE (Automatic Test Equipment) Calibration via Performance Verification at the System Interface.

T. F. Leedy. Oct 85, 5p
Included in Proceedings of Seminar on Digital Methods in Waveform Metrology, pA50-A54 Oct 83.

Keywords: Gallium arsenides, Photoconductivity, Substrates, Pulse generators, *Optoelectronic switches.

The paper describes the design of a set of optoelectronic switches having an interdigitated electrode structure and implemented with high resistivity GaAs photoconductive substrates. A theoretical analysis is developed for determining the pulsed light ON state resistance (peak conductance), OFF state (dark) resistance, and the associated capacitances for the various designed gap geometries. Data are provided on the processing steps used in successfully fabricating a working set of switches based on the theoretical design. A test apparatus is used to make measurements of the pulsed light conductance of these devices having nominal gap spacing of 5, 10, 20, and 40 micrometers.

500,655
PB86-139953

Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div.

Amplification by a Voltage Locked Array of Josephson Junctions.

Final rept.,
D. G. McDonald, and N. V. Frederick. Sep 85, 3p
Pub. in Applied Physics Letters 47, n5 p530-532, 1 Sep 85.

Keywords: *Amplifiers, Josephson junctions, Superconductivity, Reprints.

The authors have studied a new type of Josephson junction amplifier which is based on a two-junction array; the junctions are mutually phase locked at the Josephson self-oscillation frequency. With the frequency at 82 GHz, the voltages of the junctions remain equal (locked) for a bias current range as large as 60% of the critical current. Over a much smaller bias range, with an applied signal frequency of 1 kHz, a small-signal power gain of 19 dB was measured, accompanied by a negative resistance input impedance. The performance is consistent with a quasistatic theory of the amplifier.

500,656
PB86-139961

Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div.

Amplification by the Phase-Locking Mechanism in a Four-Junction SQUID.

Final rept.,
D. G. McDonald. Dec 84, 3p
Pub. in Applied Physics Letters 45, n11 p1243-1245, 1 Dec 84.

Keywords: *Amplifiers, Josephson junctions, Microwaves, Superconductivity, Reprints, SQUID devices.

It is shown that the phase-locking property of an array of Josephson junctions can be used as a basis for amplification. The particular device simulated is a superconducting quantum interference device (SQUID) with four junctions in the loop, rather than the usual one or two. Novel consequences of the design are that it allows direct rather than inductive coupling to the SQUID and, because of its potentially compact form, it probably can have a bandwidth well into the gigahertz range, in agreement with the simulations.

500,657

PB86-166634 PC A03/MF A01

National Bureau of Standards (NEL), Gaithersburg, MD. Semiconductor Electronics Div.

CSFIT: A FORTRAN Program for Charge-Sheet Model Fitting of MOSFET Data.

L. C. Witte. Nov 85, 38p NBSIR-85/3145
Sponsored by Defense Nuclear Agency, Washington, DC.

Keywords: *Metal oxide transistors, *Field effect transistors, *Computer programs, Electric current, Electric potential, Fortran, *MOSFET, CSFIT computer program, Charge sheet model, Voltage.

A FORTRAN program, CSFIT, has been developed for fitting an expression for the current-voltage (I-V) characteristics of a long-channel MOSFET to experimental I-V curves. The one-dimensional charge-sheet model developed by Brews provides the basis for the I-V characteristics. The I-V characteristics given by this model are optimized with respect to a set of experimental data using the flatband voltage and the mobility as the only adjustable parameters. The program is written so that multiple sets of I-V data can be fit simultaneously if desired. The user must supply, in specified formats, a current-voltage data file, a device parameter file, and a starting value file.

9B. Computers

500,658

FIPS PUB 1-2 PC\$20.40

National Bureau of Standards, Gaithersburg, MD.

Code for Information Interchange, Its Representations, Subsets, and Extensions.

Final rept.,
J. L. Little. c1984, 93p
Supersedes FIPS PUB 1-1.
Three ring vinyl binder also available, North American Continent price \$6.25; all others write for quote.

Keywords: *Coding, Standards, Information systems, Data processing, Computer systems hardware, National government, *Federal information processing standards, *Information interchange, Software, Communication networks, Data systems, Computer codes, Data file.

The publication provides a standard coded character set and a recommended collating sequence, subsets, extensions, and certain graphic representations for the set, all for use in Federal information processing systems, communications systems, and related equipment, that are procured by the Federal Government. This Federal Information Processing Standard adopts in whole three voluntary industry standards: a. American National Standard X3.4-1977, Code for Information Interchange (ASCII). b. American National Standard X3.32-1973, Graphic Representation of the Control Characters of American National Standard Code for Information Interchange. c. American National Standard X3.41-1974, Code Extension Techniques for Use with the 7-Bit Coded Character Set of American National Standard Code for Information Interchange. Twenty-seven other related international, national, and Federal standards are also listed.

500,659

FIPS PUB 108 PC A02

National Bureau of Standards, Gaithersburg, MD.

Alphanumeric Computer Output Microform Quality Test Slide. Category: Hardware Standard. Subcategory: Media.

Federal information processing standards (Final),
T. C. Bagg. c1983, 13p
See also FIPS PUB 82. Prepared in cooperation with Association for Information and Image Management, Silver Spring, MD.
Three ring vinyl binder also available, North American Continent price \$6.25; all others write for quote.

Keywords: *Microfilm, National government, Standards, Reprography, Data storage devices, Micrography, Inspection, Quality control, *Federal information processing standards, *Computer output microfilm, Alphanumeric data.

This FIPS PUB announces the adoption of the Association for Information and Image Management Standard for Alphanumeric COM Quality Test Slide, AIIM

MS28-1983, as a Federal standard. This standard is a companion to FIPS PUB 82, Guideline for Inspection and Quality Control for Alphanumeric Computer-Output Microforms. This standard provides detailed information for the preparation of a test form slide to ensure the generation of quality microforms by computers.

500,660

FIPS PUB 109 PC E08

National Bureau of Standards, Gaithersburg, MD.

Pascal Computer Programming Language. Category: Software Standard. Subcategory: Programming Language.

Federal information processing standards (Final),
M. V. Vickers. c1985, 133p
Three ring vinyl binder also available, North American Continent price \$6.25; all others write for quote.

Keywords: *Programming languages, Standards, *PASCAL programming language, *Federal information processing standards, Computer software, Computer program portability.

The publication announces the adoption of American National Standard Pascal Computer Programming Language, ANSI/IEEE770X3.97-1983, as a Federal Information Processing Standard (FIPS). The American National Standard Pascal, ANSI/IEEE770X3.97-1983, specifies the form and establishes the interpretation of programs expressed in the Pascal programming language. The purpose of the standard is to promote portability of Pascal programs for use on a variety of data processing systems. The standard is used 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 of the standard. (Copyright (c) 1983, American National Standards Institute, Inc., and Institute of Electrical and Electronics Engineers, Inc.)

500,661

FIPS PUB 110 PC A03/MF A01

National Bureau of Standards, Gaithersburg, MD.

Guideline for Choosing a Data Management Approach. Category: Software. Subcategory: Data Management Applications.

Federal information processing standards (Final),
J. C. Collica. 11 Dec 84, 31p
Three ring vinyl binder also available, North American Continent price \$6.25; all others write for quote.

Keywords: *Data processing, Decision making, Guidelines, *Federal information processing standards, *Data management, Data management systems, Data base management systems, File management systems.

This Guideline assists the Federal data processing manager in the identification and selection of a data management approach appropriate to organizational requirements. In this Guideline is a framework for comparing and selecting alternative data management approaches. The emphasis is on pragmatic guidance that captures the principal, relevant decision factors.

500,662

FIPS PUB 111 PC A03

National Bureau of Standards, Gaithersburg, MD.

Storage Module Interfaces (with Extensions for Enhanced Storage Module Interfaces). Category: Hardware Standard. Subcategory: Interface.

Federal information processing standards (Final),
W. E. Burr. c1982, 48p
Prepared in cooperation with American National Standards Inst., New York.
Three ring vinyl binder also available, North American Continent price \$6.25; all others write for quote.

Keywords: *Magnetic disks, *Computer storage devices, Specification, Government procurement, *Federal information processing standards, *Disk recording systems, Control units(Computers), Modules(Electronics), Storage module.

The Federal Information Processing Standard (FIPS) specifies the functional, electrical and mechanical properties of a 'device level' interface between a magnetic disk drive and its controller. The Storage Module or 'SMD' interface is very widely used in commerce, and this FIPS may be used to assist procuring agencies in the specification of interchangeable commodity magnetic disk drives and controllers. This FIPS adopts

Field 9—ELECTRONICS AND ELECTRICAL ENGINEERING

Group 9B—Computers

American National Standard, X3.91M-1982, 'Storage Module Interfaces.'

500,663
FIPS PUB 113 PC A02/MF A01
National Bureau of Standards, Gaithersburg, MD.
Computer Data Authentication. Category: ADP Operations. Subcategory: Computer Security.
Federal information processing standards (Final), M. E. Smid, and D. K. Branstad. 30 May 85, 11p
Three ring vinyl binder also available, North American Continent price \$6.25; all others write for quote.

Keywords: Authentication, Standards, *Data integrity, *Data encryption, *Federal Information Processing Standard, Computer codes, Cryptography.

The publication specifies a standard to be used by Federal organizations which require that the integrity of computer data be cryptographically authenticated. In addition, it may be used by any organization whenever cryptographic authentication is desired. Cryptographic authentication of data during transmission between electronic components or while in storage is necessary to maintain the integrity of the information represented by the data. The standard specifies a cryptographic authentication algorithm for use in ADP systems and networks. The authentication algorithm makes use of the Data Encryption Standard (DES) cryptographic algorithm as defined in Federal Information Processing Standard 46 (FIPS PUB 46).

500,664
FIPS PUB 19-1 PC A04/MF A01
National Bureau of Standards, Gaithersburg, MD.
Catalog of Widely Used Code Sets. Category: Data Standards and Guidelines Subcategory: Representations and Codes.
Federal information processing standards (Final), R. G. Saltman. 7 Jan 85, 65p
Supersedes FIPS-PUB-19.
Three ring vinyl also available, North American Continent price \$6.25; all others write for quote.

Keywords: *Data processing, *Standards, *Coding, *Catalogs(Publications), Directories, *Federal Information Processing Standards, Data elements.

The catalog lists and briefly describes code sets that are in wide use in the United States and that might be useful to Federal data systems. The purpose of the catalog is to assist Federal agencies and other organizations in the selection of appropriate code sets and in the avoidance of duplication of effort. The standard format that describes each code set listed specifies code characteristics, maintenance agency, source document, and other pertinent data. This revision supersedes FIPS PUB 19 in its entirety.

500,665
FIPS PUB 2-1 PC\$7.00
National Bureau of Standards, Gaithersburg, MD.
Perforated Tape Code for Information Interchange.
Final rept., J. L. Little. c1984, 18p
Supersedes FIPS PUB 2.
Three ring vinyl binder also available, North American Continent price \$6.25; all others write for quote.

Keywords: *Punched tapes, Code, Standards, Computer systems hardware, *Federal information processing standards, *Information interchange, Communication networks.

The publication provides the representation of the Code for Information Interchange, Its Representations, Subsets, and Extensions (FIPS 1-2) on perforated tape used in Federal information processing systems, communications systems, and associated equipment. The Federal Information Processing Standard adopts in whole American National Standard X3.6-1965 (reaffirmed in 1983), Perforated Tape Code for Information Interchange. Three other related standards are also listed. (Copyright (c) 1965, American Standards Association, Incorporated.)

500,666
FIPS PUB 33-1 PC A03
National Bureau of Standards, Gaithersburg, MD.
Character Set for Handprinting. Category: Hardware Standard. Subcategory: Character Recognition.
Federal information processing standards (Final), T. C. Bagg. c1982, 37p
Supersedes FIPS PUB 33.

Three ring vinyl FIPS binder also available, North American Continent price \$6.25; all others write for quote.

Keywords: *Data processing, *Standards, *Handwriting, *Symbols, *Federal information processing standards, *Optical character recognition.

This FIPS PUB announces the adoption of the American National Standard X3.45-1982, Character Set for Handprinting, as a Federal Standard. This standard provides the description, scope, and application rules for a character set for handprinting. A major purpose of this standard is to reduce the cost of data input into ADP systems which use Optical Character Recognition (OCR) equipment. This character set remains the same as the previous standard set with the exception of the Yen symbol.

500,667
PB85-152288 CP T02
National Bureau of Standards, Gaithersburg, MD.
Center for Programming Science and Technology.
Standard Abbreviations and Codes for States and Outlying Areas of the U.S. (FIPS PUB 5-1) and Counties and County Equivalents of the States of the United States and the District of Columbia (FIPS PUB 6-3).

Data file,
T. Henry. Jan 85, mag tape FIPS PUB 5-1, FIPS PUB 6-3, NBS/DF-85/006
Supersedes PB-190 119 and PB81-108623.
Source tape is in the EBCDIC or ASCII character set. This restricts preparation to 9 track one-half inch tape only. Identify recording mode by specifying density and character set. Call NTIS Computer Products if you have questions.

Keywords: *Data file, *Coding, Standards, Magnetic tapes, *Federal information processing standards, *Geocoding, States(United States), Counties.

This tape contains two files: FIPS PUB 5-1 (incl. change notices 1-4), Standard Abbreviations and Codes for States and Outlying Areas of the U.S., and FIPS PUB 6-3 (incl. change notices 1-4), Counties and County Equivalents of the States of the United States and the District of Columbia. Records in File 1 are sequenced in alphabetic order of the states (incl. D.C.), followed by the major outlying areas in alphabetic order, followed by the minor areas in alphabetic order. Progression of the numeric state code is consistent with alphabetic order of the states and major outlying areas. Minor outlying areas have no postal abbreviations and, in these cases, positions 51 and 52 of each record are blank. Records in File 2 are sequenced in alphabetic order of county name, within each state and outlying area. Progression of the numeric county code is consistent with alphabetic order of the counties within each state. States (incl. D.C.) and the major outlying areas are sequenced as in File 1. Minor outlying areas do not appear in File 2, as they have no county equivalent.

500,668
PB85-152312 CP T02
National Bureau of Standards, Gaithersburg, MD.
Center for Programming Science and Technology.
Codes for Named Populated Places, Primary County Divisions, and Other Locational Entities of the United States (FIPS PUB 55), 7th Update.
Data file,
H. Tom. Jan 85, mag tape FIPS PUB 55, NBS/DF-85/005
Supersedes PB84-162742.

Source tape is in the EBCDIC or ASCII character set. This restricts preparation to 9 track, one-half inch tape only. Identify recording mode by specifying density and character set. Call NTIS Computer Products if you have questions. Includes FIPS PUB 55 User Guide.

Keywords: *Data file, *Coding, *United States, Urban areas, Rural areas, Municipalities, Communities, Magnetic tapes, *Federal information processing standards, *Geocoding, Counties, ZIP codes.

This seventh update of the Federal Information Processing Standard (FIPS) 55 data file provides a two-character State code and five-character numeric place code to uniquely identify each listed entity. Areas of the United States covered are the fifty States, the District of Columbia, and all outlying territories with significant self-administration. An exhaustive list is carried of incorporated places, census designated places (CDP's), primary county divisions (such as townships, New England towns, and census county divisions),

recognized Indian reservations and Alaska Native villages, and counties. The listing also includes unincorporated places, military bases, National parks, airports, and ground transportation points. A two-character class code distinguishes over severity entity types. Each entity is identified by the county or counties in which it is located. All exhaustive categories and military bases are identified by Congressional (99th) District and by all new metropolitan statistical areas. Incorporated places, CDP's, and Indian and Alaska Native areas, are cross-referenced to U.S. Bureau of the Census files. ZIP codes are provided for all Post Offices.

500,669
PB85-161115 CP T02
National Bureau of Standards, Gaithersburg, MD.
Center for Programming Science and Technology.
MSA: Metropolitan Statistical Areas Data Tape, February 1985 Version.

Data file,
H. Tom. Feb 85, mag tape NBS/DF-85/007
Supersedes PB84-121367.
Source tape is in the ASCII or EBCDIC character set. This restricts preparation to 9 track, one-half inch tape only. Identify recording mode by specifying character set and density. Call NTIS Computer Products if you have questions.

Keywords: *Data file, *Metropolitan areas, *Coding, *Urban areas, Magnetic tapes, *Standard Metropolitan Statistical Areas, *Federal information processing standards, Geographical areas.

The Office of Management and Budget (OMB) announced revised definitions of the nation's metropolitan statistical areas (MSAs) effective June 30, 1983. Based on demographic data derived from the 1980 decennial census, a comprehensive review was undertaken by the Federal Committee on MSAs, which advises OMB on MSA matters. The previous term 'Standard Metropolitan Statistical Area (SMSA)' has been shortened to 'Metropolitan Statistical Area' (MSA). Under the new standards, an area qualifies for recognition as an MSA in one of two ways: if there is a city of at least 50,000 population, or an urbanized area of at least 50,000 with a total metropolitan population of at least 100,000. If an area has more than 1 million population and meets certain other specified requirements, it now will be termed a 'Consolidated Metropolitan Statistical Area' (CMSA), consisting of major components recognized as 'Primary Metropolitan Statistical Areas' (PMSAs). A total of 257 MSAs are recognized. In addition, there are 23 CMSAs, consisting of 78 PMSAs. This tape contains computer files documenting titles, components and Federal Information Processing Standards (FIPS) codes for Metropolitan Statistical Areas and related statistical areas. It includes two computer files to convert titles, components, and FIPS codes for Standard Metropolitan Statistical Areas to June 30, 1983 MSA definitions.

500,670
PB85-170595 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Mathematical Software for Elliptic Boundary Value Problems.
Final rept.,
R. F. Boisvert, and R. A. Sweet. 1984, 64p
Pub. in Chapter 9 in Sources and Development of Mathematical Software, p200-263 1984.

Keywords: *Partial differential equations, *Elliptic differential equations, *Boundary value problems, *Numerical integration, Reprints, *Computer software, Software engineering.

The authors survey recent advances in general-purpose mathematical software for elliptic partial differential equations. First, the types of equations handled by extant software are characterized and the most popular numerical methods are outlined. They then discuss software engineering issues related to the design and production of high-quality software which implement these methods. Detailed case studies are presented for two software packages: ELLPACK and FISHPAK. The authors conclude with a catalog of currently available software, describing the problems solved, the numerical methods, portability, and distribution in each case.

500,671
PB85-170637 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.

Fiber Distributed Data Interface: A Proposal for a Standard 100 Mbit/s Fiber Optic Token Ring Network.

Final rept.,
W. E. Burr, and F. E. Ross. Sep 84, 4p
Prepared in corporation with Sperry Corp., Blue Bell, PA.
Pub. in Proceedings of FOC/LAN 1984, Las Vegas, Nevada, September 17-21, 1984, p254-257.

Keywords: *Computer networks, *Fiber optics, *Standards, *Local area networks.

The Fiber Distributed Data Interface, a proposed American National Standard for a 100 Mbit/s token ring network using optical fiber, is described. The purpose of this proposed standard is the interconnection of a number of high performance mainframe computers or supercomputers, together with mass storage elements, to form a loosely-coupled system in a local network (that is building or campus-wide) environment.

**500,672
PB85-177632 PC A04/MF A01**

National Bureau of Standards, Gaithersburg, MD. Center for Programming Science and Technology. **Guide on Workload Forecasting.**
Final rept.,
H. Letmanyi. Mar 85, 71p NBS/SP-500/123
Also available from Supt. of Docs as SN003-003-02634-4. Library of Congress catalog card no. 85-600504.

Keywords: *Data processing, *Forecasting, *Work measurement, Time series analysis, *Data base administrators, *Data base management systems, *Workload.

The purpose of this guide is to provide ADP managers and technical personnel with useful quantitative techniques for forecasting future workload requirements. It additionally provides a step-by-step approach to the forecasting process. Readers can then, in a timely manner, provide the computing resources needed to perform the user's workload at required service levels throughout the life-cycle of an ADP system. These techniques are described so that readers with little or no training in statistics should find them useful. However, this guide does not intend to give an exhaustive treatment of the techniques discussed. Readers requiring more information are referred to Appendix A ('Suggested Readings and References').

**500,673
PB85-177657 PC A04/MF A01**

National Bureau of Standards, Gaithersburg, MD. Systems and Network Architecture Div. **Performance Measurement of OSI (Open System Interconnection) Class 4 Transport Implementations.**
K. L. Mills, J. W. Gura, and C. M. Chernick. Jan 85, 53p NBSIR-85/3104

Keywords: *Computer networks, Performance evaluation, Measurement, Implementation, *Protocols, Open system interconnections.

A measurement system to evaluate the performance of open system interconnection (OSI) transport protocol implementations is described. Several metrics are proposed to establish a quantitative characterization of layered protocol performance. Metrics specific to the OSI transport protocol are also proposed. The measurement system and metrics are applied to a multi-vendor National Computer Conference demonstration network and the results are reported.

**500,674
PB85-177970 PC A05/MF A01**

National Bureau of Standards, Gaithersburg, MD. Center for Programming Science and Technology. **Guide on Logical Database Design.**
Final rept.,
E. N. Fong, M. W. Henderson, D. K. Jefferson, and J. M. Sullivan. Feb 85, 119p NBS/SP-500/122
Also available from Supt. of Docs as SN003-003-02631-0. Library of Congress catalog card no. 85-600500.

Keywords: *Information systems, Systems design, Systems analysis, Methodology, *Data base design, *Data bases, *Data management, *Data base management systems, Data dictionaries, User needs, Relational data base.

This report discusses an iterative methodology for Logical Database Design. The methodology includes

four phases: Local Information-flow Modeling, Global Information-flow Modeling, Conceptual Schema Design, and External Schema Modeling. These phases are intended to make maximum use of available information and user expertise, including the use of a previous Needs Analysis, and to prepare a firm foundation for physical database design and system implementation. The methodology recommends analysis from different points of view--organization, function, and event--in order to ensure that the logical database design accurately reflects the requirements of the entire population of future users. The methodology also recommends computer support from a data dictionary system, in order to conveniently and accurately handle the volume and complexity of design documentation and analysis. The report places the methodology in the context of the complete system life cycle. An appendix of illustrations shows examples of how the four phases of the methodology can be implemented.

**500,675
PB85-177996 PC A04/MF A01**

National Bureau of Standards, Gaithersburg, MD. Inst. for Computer Sciences and Technology. **Guidance on Planning and Implementing Computer System Reliability.**
Final rept.,
L. S. Rosenthal. Jan 85, 53p NBS/SP-500/121
Also available from Supt. of Docs as SN003-003-02628-0. Library of Congress catalog card no. 84-601159.

Keywords: *Systems management, Computers, Reliability, Specifications, Measurement, Quality, Projects, *Computer system reliability, *Computer system design, Systems engineering.

Computer systems have become an integral part of most organizations. The need to provide continuous, correct service is becoming more critical. However, decentralization of computing, inexperienced users, and larger more complex systems make for operational environments that make it difficult to provide continuous, correct service. This document is intended for the computer system manager (or user) responsible for the specification, measurement, evaluation, selection or management of a computer system. This report addresses the concepts and concerns associated with computer system reliability. Its main purpose is to assist system managers in acquiring a basic understanding of computer system reliability and to suggest actions and procedures which can help them establish and maintain a reliability program. The report presents discussions on quantifying reliability and assessing the quality of the computer system. Design and implementation techniques that may be used to improve the reliability of the system are also discussed. Emphasis is placed on understanding the need for reliability and the elements and activities that are involved in implementing a reliability program.

**500,676
PB85-183572 Not available NTIS**

National Bureau of Standards, Gaithersburg, MD. **Integrity and Security Standards Based on Cryptography.**
Final rept.,
D. K. Branstad, and M. E. Smid. 1982, 6p
Pub. in Computer Security 1, n3 p255-260 Nov 82.

Keywords: Security, Standards, Reprints, *Computer security, *Data Encryption Standard, *Cryptography, Federal Information Processing Standard, Authentication.

Since the Data Encryption Standard (DES) was published in January 1977, as a Federal Information Processing Standard (FIPS), it has become the basis for the development of several security and integrity standards. Seven DES based security standards have already been approved, and several others are in development. Five standards making organizations are now involved with DES based standards: the American Bankers Association (ABA), the American National Standards Institute (ANSI), the General Services Administration (GSA), the International Organization for Standardization (ISO), and the National Bureau of Standards (NBS). While these standards are all based on the DES, future standards may make provision for using other cryptographic algorithms. For example, public key cryptographic algorithms could offer some advantages over the traditional, secret key cryptographic algorithms in certain applications. In anticipation of this future requirement NBS has published a Solicitation for Public Key Cryptographic Algorithms to be based in special application standards.

**500,677
PB85-191385 PC A02/MF A01**

National Bureau of Standards, Gaithersburg, MD. Inst. for Computer Sciences and Technology. **Annotated Bibliography of Recent Papers on Software Engineering Environments.**
Final rept.,
R. C. Houghton, and D. R. Wallace. Apr 85, 25p
NBSIR-85/3113

Keywords: *Computer programming, *Bibliographies, Environments, Requirements, *Software engineering, Software tools, Interactive systems.

This document reports on the contents of fifty-five recent papers on software engineering environments. Several of these papers present an overview of software engineering environments. Other papers discuss issues to be considered in building software engineering environments. The remaining papers describe general software engineering environments, system development environments, and programming environments.

**500,678
PB85-191955 PC A04/MF A01**

National Bureau of Standards (NML), Gaithersburg, MD. Office of Standard Reference Data. **PIPE/1000: An Implementation of Piping on an HP-1000 Minicomputer.**
Final rept.,
N. L. Seidenman. Mar 85, 54p NBS/TN-1208
Also available from GPO as SN003-003-02639-5.

Keywords: *Operating systems(Computers), *Routing, Computer programs, Linkages, Implementation, Minicomputers, *PIPE system, *UNIX system, C programming language.

Piping is a system by which programs can communicate so as to coordinate their respective functions in a synchronized effort aimed at the completion of a given task. Piping is one of the strong points of the increasingly popular operating system UNIX, developed at Bell Laboratories and licensed by AT&T. This paper describes an implementation of piping in a non-UNIX environment; in particular, on an HP-1000 minicomputer.

**500,679
PB85-197747 Not available NTIS**

National Bureau of Standards, Gaithersburg, MD. **Mathematical Software in Basic.**
Final rept.,
D. K. Kahaner, and W. L. Wyman. 1983, 5p
Pub. in IEEE (Institute of Electrical and Electronics Engineers) Micro. 3, n5 p42-46 Oct 83.

Keywords: BASIC programming language, Numerical quadrature, Approximation, Algorithms, Reprints, *Integrals, *Computer software, One dimensional.

A new algorithm is presented for approximation of one dimensional definite integrals. It is implemented in Basic.

**500,680
PB85-201796 Not available NTIS**

National Bureau of Standards, Gaithersburg, MD. Data Management and Programming Languages Div. **Tour of Computing Facilities in China.**
Final rept.,
H. M. Wood, D. J. Reifer, and M. Sloan. Jan 85, 8p
Pub. in Computer 18, n1 p80-87 Jan 85.

Keywords: *China, Computers, Facilities, Asia, Reprints, *Computer applications, *Technology utilization.

The First International Conference on Computers and Applications was held in Beijing, China, June 20-22, 1984. This report describes visits made to various computing-related sites in Beijing and Shanghai by three attendees from the conference. Its intention is to provide some representative examples of present computer use and some indicators of China's current priorities and strategies for harnessing that technology.

**500,681
PB85-202018 Not available NTIS**

National Bureau of Standards, Gaithersburg, MD.

Field 9—ELECTRONICS AND ELECTRICAL ENGINEERING

Group 9B—Computers

Reflections on Ten Years of Computer Security.

Final rept.,
S. K. Reed, and D. K. Branstad. 1982, 2p
Pub. in Computing Security 1, n3 p231-232 Nov 82.

Keywords: Risk, Verifying, Reprints, *Computer security, *Data encryption, Access.

The progress in computer security in the last ten years is considered from the standpoint of what has and has not changed.

500,682

PB85-202158 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Scientific Computing Div.
Survey of Mathematical Software for Elliptic Boundary Value Problems.

Final rept.,
R. F. Boisvert, and R. A. Sweet. 1982, 3p
Sponsored by International Association for Mathematics and Computers in Simulation and Concordia Univ., Loyola Campus, Montreal (Quebec).
Pub. in Proceedings of World Congress on System Simulation and Scientific Computation (10th), Montreal, Canada, August 8-13, 1982, Numerical Methods for Scientific Computation, v1, p449-451 1982.

Keywords: *Boundary value problems, *Elliptic differential equations, *Partial differential equations, Reviews, *Computer software.

In this paper, the authors summarize the state of mathematical software for elliptic boundary value problems. These problems are fundamental to the study of static physical phenomena such as electromagnetic fields and steady-state diffusion. In addition, they often arise as intermediate steps in the modelling of dynamic processes such as fluid flow. The authors limit this discussion to portable general-purpose mathematically-oriented software, and hence much useful applications-oriented is necessarily omitted.

500,683

PB85-202919 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Systems and Software Technology Div.
Structural Dimensions of Small Programming Environments.
Final rept.,
G. Lyon. Jan 85, 13p
Pub. in Jnl. of Software--Practice and Experience 15, n1 p105-117 Jan 85.

Keywords: *Computer programming, Reprints, *Computer software.

Although substantial variety exists among small programming environments, common points-of-choice in their design suggest the following structural characterization: real or virtual hardware; message-passing or procedure-calling; static or dynamic binding; horizontal or vertical organizations; abstract or concrete structures; fixed or extensible language. Often these dimensions must support a very focused programming idiom, which combined with other requirements such as portability or performance, establishes structural dependencies, precludes features and forces exceptions. The characterization provides a rough framework that is useful in evaluating programming environments.

500,684

PB85-202935 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
View of Software Development Support Systems.
Final rept.,
M. A. Branstad, W. R. Adron, and J. C. Cherniavsky. 1981, 6p
Sponsored by National Engineering Consortium, Inc., Oak Brook, IL.
Pub. in Proceedings of Natl. Electronics Conf., Chicago, IL, October 26-28, 1981, v35, p257-262.

Keywords: *Systems engineering, Computer programming, Automation, *Computer software, *Software engineering.

The ability to adequately monitor and control the software development process is important as a mechanism for achieving higher quality and productivity. Automation, specifically a collection of software development tools, can be used to facilitate and constrain the process. Integrated tool collections are termed software development support systems on programming environments.

500,685

PB85-221950 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Database Management in Science and Technology.
Final rept.,
J. Rumble. 1984, 14p
Pub. in Database Management in Science and Technology, p1-13 1984.

Keywords: Computation, *Data base management, Science and technology, Numerical data, Computer systems design.

The paper features an introduction to the use of computers in the handling of numeric scientific data. It is the introductory chapter in a new CODATA Sourcebook. In addition, it outlines the use of database management systems and their design.

500,686

PB85-221968 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Analysis and Display of Data in Science and Technology.
Final rept.,
J. R. Rumble, and N. L. Seidenman. 1984, 17p
Pub. in Database Management in Science and Technology, p75-91 1984.

Keywords: Computation, Statistical analysis, Data displays, Photocomposition, Bibliographies, *Data base management, Numerical data, Computer graphics, Data analysis, Science and technology.

The paper discusses the use of numeric databases including preparation of subsets, statistical analysis, photocomposition, and graphics. Examples of each are given as well as a comprehensive bibliography.

500,687

PB85-224491 PC A07/MF A01
National Bureau of Standards, Gaithersburg, MD. Center for Programming Science and Technology.
Technical Overview of the Information Resource Dictionary System.
A. Goldfine, and P. Konig. Apr 85, 135p NBSIR-85/3164

Keywords: Standardization, Specifications, Proposals, *Data base management, *Information Resource Dictionary System, *IRDS system, *Federal information processing standards, Information processing, Computer software, Data dictionary, International standard.

The publication provides a technical overview of the computer software specifications for an Information Resource Dictionary System (IRDS). It summarizes the data architecture and the software functions and processes of the IRDS. The IRDS Specifications are a draft proposed American National Standard, a draft proposed U.S. Federal Information Processing Standard, and a Working Document of the International Organization for Standardization (ISO), Subcommittee 21, Working Group 3. The Overview also provides background information on the development of the draft proposed U.S. standards.

500,688

PB85-225217 PC A05/MF A01
National Bureau of Standards, Gaithersburg, MD.
Reference Model for DBMS (Database Management System) Standardization.
D. K. Jefferson, and E. N. Fong. May 85, 79p
NBSIR-85/3173

Keywords: Standardization, Models, Concepts, Proposals, *Data management, *Data base management systems, *DBMS systems, *Data dictionary, Reference models, Data representation, DL programming language, i-DL programming language.

The report proposes a Reference Model (RM) for database management system (DBMS) standardization. A Reference Model is a conceptual framework whose purpose is to divide standardization work into manageable pieces and to show at a general level how these pieces are related with each other. The proposed RM comprises a Data Mapping Control System (DMCS) that retrieves and stores application data, application schemas, and data dictionary schemas. This DMCS is bounded by two interfaces: the Data Language (DL) interface which defines the services offered by the DMCS to various Data Management Tools (DMT), and the internal Data Language (i-DL) interface which de-

finer the services required by the DMCS from the host operating system. The report suggests two candidates for standardization: the DL and the i-DL.

500,689

PB85-227783 PC A05/MF A01
National Bureau of Standards, Gaithersburg, MD. Center for Programming Science and Technology.
Using the Information Resource Dictionary System Command Language.
Final rept.,
A. Goldfine. Apr 85, 86p NBSIR-85/3165

Keywords: *Information systems, *Data base management systems, *Command languages, *Data dictionary, Information Resource Dictionary System, IRDS system.

The document introduces and provides examples of the Command Language of the draft proposed Information Resource Dictionary System (IRDS). A dictionary maintained by the U.S. Air Force is defined in the IRDS and used as a continuing example throughout the document. The dictionary is populated, manipulated; and reported on using the precise syntax of the Command Language. An appendix to the document provides a complete listing of the creation of the example. Other appendices provide indices of all command appearances and all clause appearances.

500,690

PB85-238244 PC A12/MF A01
National Bureau of Standards, Gaithersburg, MD. Inst. for Computer Sciences and Technology.
Workshop on Analytic and Simulation Modeling of IEEE 802.4 Token Bus Local Area Networks Held at Gaithersburg, Maryland on April 29-30, 1985.
Final rept.,
R. Rosenthal. Jun 85, 270p NBS/SP-500/127
See also PB85-238251 through PB85-238418. Also available from Supt. of Docs as SN003-003-02660-3. Library of Congress catalog card no. 85-600556.

Keywords: *Computer networks, Standards, Simulation, Meetings, *Token bus networks, *Local area networks.

Token bus Local area networking technology is anticipated for use by national and international organizations seeking standard solutions for process control and Laboratory and factory automation applications. Several token passing technologies have been described; but, only one emerging standard, the IEEE 802.4 Token Bus currently includes broadband communications utilizing a prioritized, robust and deterministic access method. The workshop proceedings report the deliberations of 39 participants from industry, academia, and the Federal Government who came to NBS to (1) encourage modeling of 802.4, (2) to build competence and confidence in 802.4 technology, (3) to provide public knowledge about the behavior, characteristics and performance of 802.4 and to highlight areas for further study on the NBS 802.4 test bed facility.

500,691

PB85-238251
(Order as PB85-238244, PC A12/MF A01)
National Bureau of Standards, Gaithersburg, MD. Inst. for Computer Sciences and Technology.
Analytic and Simulation Modeling of IEEE 802.4 Token Bus.
R. Rosenthal. Jun 85, 2p
Included in Workshop on Analytic and Simulation Modeling of IEEE 802.4 Token Bus Local Area Networks, p2-3 Jun 85.

Keywords: *Computer networks, Standards, Simulation, Meetings, *Token bus networks, *Local area networks.

Token bus technology is anticipated for use by national and international organizations seeking standard local area network solutions for factory, laboratory and process control automation applications. Several token passing technologies have been described; but, only one emerging token bus standard, the IEEE 802.4 Token Bus, currently includes broadband facilities.

500,692

PB85-238269
(Order as PB85-238244, PC A12/MF A01)
GMI Engineering and Management Inst., Flint, MI.

Performance Simulation of the IEEE Token Bus Protocol Using SIMAN,

J. R. Pimentel. Jun 85, 31p

Included in Workshop on Analytic and Simulation Modeling of IEEE 802.4 Token Bus Local Area Networks, p5-35 Jun 85.

Keywords: *Computer networks, Standards, Simulation, Meetings, *Token bus networks, *Local area networks.

The SIMAN simulation language is used to simulate the performance of the physical and data link layers of a local area network suitable for manufacturing. The protocol standards specified by the IEEE project 802.4 has been chosen for the study. A detailed network queueing model is developed and implemented using the process view approach provided by SIMAN. Simulation results are shown in terms of average number of frames awaiting transmission, average response time, and medium utilization versus traffic intensity.

500,693

PB85-238277

(Order as PB85-238244, PC A12/MF A01)

Boeing Computer Services Co., Seattle, WA.

Discrete Event Simulation of the IEEE 802.4 Token Bus LAN (Local Area Networks) Protocol: A Structured Analysis Approach,

E. R. Nugent. Apr 85, 17p

Included in Workshop on Analytic and Simulation Modeling of IEEE 802.4 Token Bus Local Area Networks, p35-51 Jun 85.

Keywords: *Computer networks, Standards, Simulation, Meetings, *Token bus networks, *Local area networks.

Boeing Computer Services is developing a discrete event simulation of the IEEE 802.4 Token Bus Media Access Control protocol. NBS will use the simulation model as part of their token bus research project. The paper describes the BCS simulation approach. Topics include project background, objectives and the simulation methodology used.

500,694

PB85-238285

(Order as PB85-238244, PC A12/MF A01)

Rockwell International, Thousand Oaks, CA. Science Center.

Simulation of the IEEE 802.4 Token Passing Bus Protocol Using SIMSCRIPT,

A. R. K. Sastry, and M. W. Atkinson. Jun 85, 9p

Included in Workshop on Analytic and Simulation Modeling of IEEE 802.4 Token Bus Local Area Networks, p52-61 Jun 85.

Keywords: *Computer networks, Standards, Simulation, Meetings, SIMSCRIPT, *Token bus networks, *Local area networks.

A simulation model has been developed for the performance evaluation of the IEEE 802.4 token passing bus local area network protocol using SIMSCRIPT. The model has identifiable 'processes' corresponding to the four 'machines' of the protocol, i.e., access control, receive, transmit, and interface machines. In addition, a 'frame process' is used to simulate the signal flow on the bus. An initialization 'routine' serves to input the network parameters and to initially activate the processes in the proper order, while a statistics extraction routine gathers output data during a simulation run. The entire model is developed in an incremental mode, gradually increasing the detail and complexity so that code can be validated by 'walking through' at every stage of the development. Queues with four different priorities, a message generation process at each queue, random selection of frame lengths, and token rotation timers have been incorporated. Results from a number of simulation runs suggest the need to develop methodology to relate the timer values with the desired priorities under given traffic conditions, which seems to be a very significant user-oriented issue.

500,695

PB85-238293

(Order as PB85-238244, PC A12/MF A01)

Motorola Semiconductor Israel Ltd., Ramat-Gan.

Token Bus (IEEE Std. 802.4) Network Simulator,

O. Kremien. Jun 85, 7p

Included in Workshop on Analytic and Simulation Modeling of IEEE 802.4 Token Bus Local Area Networks, p62-68 Jun 85.

Keywords: *Computer networks, Standards, Simulation, Meetings, *Token bus networks, *Local area networks.

The Token Bus Network Simulator (TBNS), developed by Motorola Semiconductor Israel (MSIL), is a software tool which aids in Token-Bus (IEEE 802.4) protocol developments, verification and performance evaluation. It is a discrete event-driven simulator that is coded in PASCAL and provides predictions of delay, throughput and many other performance measures as a function of offered load. The simulator implements the IEEE 802.4 (Rev. A, 1984) Token-Passing Bus Medium Access Control (MAC) Specification of protocols for local area networks. It models token-bus network behavior in batch mode and under interactive user control (MAC) Specification of protocols for local area networks. It models token-bus network behavior in batch mode and under interactive user control. The simulator can trace the progress through the network of each message/event to facilitate model validation and analysis. Use of the simulator at MSIL has resulted in the discovery of several protocol errors (including one deadlock situation) which were reported back to the IEEE 802.4 committee.

500,696

PB85-238301

(Order as PB85-238244, PC A12/MF A01)

Industrial Technology Inst., Ann Arbor, MI. Communications and Network Lab.

Performability Modeling Tools,

J. F. Meyer. Jun 85, 33p

Included in Workshop on Analytic and Simulation Modeling of IEEE 802.4 Token Bus Local Area Networks, p69-101 Jun 85.

Keywords: *Computer networks, Performance evaluation, Standards, Simulation, Meetings, *Token bus networks, *Local area networks.

Methods/tools for modeling performability (unified performance-reliability) are described with application to the evaluation of real-time local area networks. Emphasis is placed on the use of stochastic activity networks (SANs), where the presentation includes precise definitions of a SAN and associated concepts. Construction of SAN-based performability models is then discussed and the use of the procedure is illustrated in the modeling of a local area network with timing constraints.

500,697

PB85-238319

(Order as PB85-238244, PC A12/MF A01)

National Bureau of Standards, Gaithersburg, MD. Inst. for Computer Sciences and Technology.

Token Passing Networks and Starvation Issues,

A. Nakassis. Jun 85, 10p

Included in Workshop on Analytic and Simulation Modeling of IEEE 802.4 Token Bus Local Area Networks, p102-112 Jun 85.

Keywords: *Computer networks, Standards, Simulation, Meetings, *Token bus networks, *Local area networks.

In the report the authors advance a necessary and sufficient condition for a low priority queue to eventually get and use the token. Then the authors will use some of the machinery they will develop in the proof of the above mentioned condition in order to explore issues of Target Rotation Time (TRT) allocation and fairness.

500,698

PB85-238327

(Order as PB85-238244, PC A12/MF A01)

Ungermann-Bass, Inc., Santa Clara, CA.

Performance Analysis of the 802.4 Token Bus Media Access Control Protocol,

J. Y. Chien. Jun 85, 41p

Included in Workshop on Analytic and Simulation Modeling of IEEE 802.4 Token Bus Local Area Networks, p113-152 Jun 85.

Keywords: *Computer networks, Standards, Simulation, Meetings, *Token bus networks, *Local area networks.

IEEE Standard 802.4--1984 defines a local area network protocol based on the concept of token-passing for controlling access to a broadcast medium. A performance analysis of such a network using simulation techniques has been conducted. Performance is characterized in terms of stability, fairness, throughput, and acquisition delay. The paper is a report on some of

those efforts. The authors analysis shows that the network remains stable as the load increases. Fairness can be attained if enough time is allowed for the system to become saturated. The acquisition delay is sensitive and degrades greatly as load increases. A comprehensive discussion of how the performance of the network is affected by system parameters like data length, network sizes, token hold time, and station delay is also included.

500,699

PB85-238335

(Order as PB85-233244, PC A12/MF A01)

Motorola, Inc., Phoenix, AZ. Semiconductor Group.

Performance Issues of 802.4 Token Bus LANs (Local Area Networks),

B. A. Loyer, and D. Kolton. Jun 85, 13p

Prepared in cooperation with Motorola Semiconductor Israel Ltd., Tel Aviv.

Included in Workshop on Analytic and Simulation Modeling of IEEE 802.4 Token Bus Local Area Networks, p153-167 Jun 85.

Keywords: *Computer networks, Standards, Simulation, Meetings, *Token bus networks, *Local area networks.

The paper presents curves generated via a software simulator that deals with several aspects of 802.4 Token Bus performance. The areas considered include dependence on station address allocation, the number of stations, the cable length, the frame length, the number of stations transmitting, and the token hold time. A brief description of the simulator is first presented and each area of performance impact is then discussed.

500,700

PB85-238343

(Order as PB85-238244, PC A12/MF A01)

General Electric Corporate Research and Development, Schenectady, NY.

Simulation of a Token Passing Bus Using a Static Logical Ring,

M. E. Ulug, and N. R. Shapiro. Jun 85, 11p

Included in Workshop on Analytic and Simulation Modeling of IEEE 802.4 Token Bus Local Area Networks, p168-179 Jun 85.

Keywords: *Computer networks, Standards, Simulation, Meetings, *Token bus networks, *Local area networks.

Process oriented and critically timed communications requirements necessitates a real-time, failure-proof network for factory automation. The ability to control the accessing at the data link level by assigning priorities and timers make token passing more advantageous in the factory environment. The performance of token passing schemes depends greatly on the value of various timers that can be controlled at the data link level. A hierarchical policy to assign values for various timers in token passing access method in an optimization framework is reported. The basic idea in the scheme is to decompose the decision making capability into two hierarchically arranged levels. In the higher level, a centralized linear programming problem is solved to maximize the overall bus utilization of the network. In the lower level, a distributed integer programming problem is solved at each station to maximize the buffer utilizations. The higher level problem is solved at a slower time scale compared to lower level problem.

500,701

PB85-238350

(Order as PB85-238244, PC A12/MF A01)

Industrial Technology Inst., Ann Arbor, MI. Communications and Network Lab.

Hierarchical Policy for Timer Assignments in IEEE 802.4 Network,

K. H. Muralidhar. Jun 85, 23p

Included in Workshop on Analytic and Simulation Modeling of IEEE 802.4 Token Bus Local Area Networks, p180-202 Jun 85.

Keywords: *Computer networks, Standards, Simulation, Meetings, *Token bus networks, *Local area networks.

Process oriented and critically timed communications requirements necessitates a real-time, failure-proof network for factory automation. The ability to control the accessing at the data link level by assigning priorities and timers make token passing more advanta-

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Group 9B—Computers

geous in the factory environment. The performance of token passing schemes depends greatly on the value of various timers that can be controlled at the data link level. A hierarchical policy to assign values for various timers in token passing access method in an optimization framework is reported. The basic idea in the scheme is to decompose the decision making capability into two hierarchically arranged levels. In the higher level, a centralized linear programming problem is solved to maximize the overall bus utilization of the network. In the lower level, a distributed integer programming problem is solved at each station to maximize the buffer utilizations. The higher level problem is solved at a slower time scale compared to lower level problem.

500,702

PB85-238368

(Order as PB85-238244, PC A12/MF A01)
National Bureau of Standards, Gaithersburg, MD. Inst. for Computer Sciences and Technology.
Stability of a Token Passing Network,
A. Nakassis. Jun 85, 14p
Included in Workshop on Analytic and Simulation Modeling of IEEE 802.4 Token Bus Local Area Networks, p203-216 Jun 85.

Keywords: *Computer networks, Standards, Simulation, Meetings, *Token bus networks, *Local area networks.

In what follows the authors study the stability of token passing networks with a fixed number of queues and they deduce the average rotation time for the token and the average user time per queue, under the assumption that the system is stable. The results will then be used to derive system parameters that will make the network stable.

500,703

PB85-238376

(Order as PB85-238244, PC A12/MF A01)
Delaware Univ., Newark. Dept. of Computer and Information Sciences.
IEEE 802.4 Token Bus Emulator,
F. Sylvanus, and T. Saydam. Jun 85, 12p
Included in Workshop on Analytic and Simulation Modeling of IEEE 802.4 Token Bus Local Area Networks, p217-228 Jun 85.

Keywords: *Computer networks, Standards, Simulation, Meetings.

A performance evaluation facility which emulates Media Access Control (MAC) portion of the IEEE 802.4 'token bus' standards is presented. The facility consists of an emulator that implements the MAC components of the token bus standards, and a representation of the physical layer of the standards as required to logically interconnect the MAC peer entities. The emulator also includes minimal implementations of the Logical Link Control and Network Management facilities as required to generate and monitor network traffic and initialize the emulator. Experiments intended to measure network delay under several network loading scenarios as a function of MAC parameters are suggested.

500,704

PB85-238384

(Order as PB85-238244, PC A12/MF A01)
National Bureau of Standards, Gaithersburg, MD. Inst. for Computer Sciences and Technology.
Notes from the Factory Automation Applications Session,
Jun 85, 5p
Included in Workshop on Analytic and Simulation Modeling on IEEE 802.4 Token Bus Local Area Networks, p230-234 Jun 85.

Keywords: *Computer networks, Standards, Simulation, Meetings, *Token bus networks, *Local area networks.

No abstract available.

500,705

PB85-238392

(Order as PB85-238244, PC A12/MF A01)
Communications and Power Engineering, Inc., Calabasas, CA.

Terminology Dictionary and Baseline Variables for IEEE 802.4 Token Bus LAN (Local Area Networks) Simulation

S. Dunford. Jun 85, 6p
Included in Workshop on Analytic and Simulation Modeling of IEEE 802.4 Token Bus Local Area Networks, p241-246 Jun 85.

Keywords: *Computer networks, Standards, Simulation, Meetings, *Token bus networks, *Local area networks.

The working paper presents a first draft of a terminology dictionary and a set of baseline variables to be used in simulation modeling of IEEE 802.4 Token Bus so as to create a basis for comparison in future workshops. It will be refined and expanded in the future. Any suggestions and criticisms should be addressed to Stephen Dunford at the above address.

500,706

PB85-238400

(Order as PB85-238244, PC A12/MF A01)
Industrial Technology Inst., Ann Arbor, MI. Communications and Network Lab.
Minutes of Special Interest Group Meeting on Conformance Testing,
K. H. Muralidhar. Jun 85, 3p
Included in Workshop on Analytic and Simulation Modeling of IEEE 802.4 Token Bus Local Area Networks, p248-250 Jun 85.

Keywords: *Computer networks, Standards, Simulation, Meetings, *Token bus networks, *Local area networks.

In the report, three main aspects of conformance testing of IEEE 802.4 protocol were discussed. The aspects discussed were, test architecture, test structure, and types of testing.

500,707

PB85-238418

(Order as PB85-238244, PC A12/MF A01)
National Bureau of Standards, Gaithersburg, MD. Inst. for Computer Sciences and Technology.
Simulation Subgroup Summary,
Jun 85, 6p
Included in Workshop on Analytic and Simulation Modeling of IEEE 802.4 Token Bus Local Area Networks, p251-256 Jun 85.

Keywords: *Computer networks, Standards, Simulation, Meetings, *Token bus networks, *Local area networks.

No abstract available.

500,708

PB85-242394

PC A03/MF A01
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Building Technology.
User's Manual for Division 746's Image Processing System,
D. P. Bentz, J. W. Martin, M. E. McKnight, E. J. Embree, and M. E. Batts. Jul 85, 33p NBSIR-85/3207
Prepared in cooperation with Paratech, Washington, DC.

Keywords: *Image processing, Image analysis, Image enhancement, User manuals, Pixels.

An image analysis system has been developed which allows the user to evaluate images in either an interactive or a batch mode. The manual provides instructions for assessing the imaging system (hardware and software) and describes the structure and function of each of the available commands. The imaging software is for an 80826 based minicomputer operating under a multi-user operating system with five imaging boards. The interactive run time environment is menu driven. To execute the imaging system in batch format, commands of a specific structure are placed into a datafile from which they are subsequently read and executed one at a time.

500,709

PB86-105814

Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Measurement Center for the NBS (National Bureau of Standards) Local Area Computer Network,
Final rept.,
P. D. Amer. 1982, 7p
Pub. in Institute of Electrical and Electronic Engineers Trans. Comput. C-31, n8 p723-729 Aug 82.

Keywords: *Computer networks, *Network flows, Performance evaluation, Radio broadcasting, *Local area networks, *NBSNET computer network, Multiple access, Distributed computer systems.

The paper describes a measurement center for a local area computer network (LAN). A LAN measurement center is a tool that allows careful testing and evaluation of a network under diverse and highly controlled conditions. Three measurement center components are discussed: a monitoring system, analysis software, and an artificial traffic generator. The monitoring system captures measurement information about the traffic being transmitted over the network. The analysis software provides ten measurement reports which are generated following each monitoring period. Finally, the traffic generator can place varied loads on the network, allowing for controlled experimentation and functional testing. The measurement center described here is being implemented for the NBSNET, a distributed, broadcast LAN at the National Bureau of Standards. Implementation issues and problems are discussed.

500,710

PB86-105855

Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Services and Mechanisms of a Data Presentation Protocol,
Final rept.,
S. E. Clopper, and J. E. Swanson. 1982, 4p
Pub. in Proceedings of INFOCOM 82, Las Vegas, Nevada, March 30-April 1, 1982, p148-151.

Keywords: *Open system interconnection, *Computer networks, *Computer files, Data requirements, Protocols.

The paper describes the services and protocol mechanisms of a protocol residing in layer six of the International Standards Organization's (ISO's) Reference Model for Open Systems Interconnection. The Data Presentation Protocol (DPP) was designed to provide presentation layer services to a File Transfer Protocol entity residing at layer seven of the ISO model. The services are consistent with the current concept of the presentation layer within ISO and the American National Standards Institute (ANSI). Specific features were selected based on the needs of the agencies of the Federal Government within the United States; however, these needs are consistent with those of any large organization engaged in the procurement or development of networks of heterogeneous computer systems.

500,711

PB86-111002

Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Systems and Software Technology Div.
Is There a Language-Knowledgeable Program Constructor-Executor in Your Future,
Final rept.,
P. B. Henderson. 1982, 1p
Pub. in Proceedings of Institute of Electrical and Electronics Engineers Computer Society's International Computer Software and Applications Conference (6th), Chicago, IL., November 8-12, 1982 p613.

Keywords: *Computer programming, Editing, Programming languages, Reprints, *Software engineering, *Personal computers, *User needs, Software tools.

The author believes that within the next 10-15 years most software development will be done on personal workstations using an environment which includes a language-knowledgeable program constructor-executor system which is tuned to the users needs.

500,712

PB86-111341

Not available NTIS
National Bureau of Standards, Boulder, CO.
Description of a Planned Federal Information Processing Standard for Data Presentation Protocol,
Final rept.,
J. R. Moulton. 1982, 6p
Pub. in Proceedings of the International Conference on Computer Communication, Pathways to the Information Society (6th), London, England, September 7-10, 1982, p896-901.

Keywords: *Computer networks, *Standards, Specifications, Procurement, *Federal Information Processing Standards, *Open system interconnection, *Data presentation protocols.

The National Bureau of Standards has developed service and design specifications for internet, transport, session, data presentation, and file transfer protocols for use in computer systems and network procurements. These protocols reside in layers three, four, five, six and seven of the International Organization for Standardization's (ISO) Reference Model of Open Systems Interconnection. This paper describes the services and internal behavior of the data presentation protocol, as well as specifications for the other protocols, was derived from the most recent developments within ISO. Specific features were selected based on the needs of the agencies of the Federal Government of the United States. These needs are consistent with those of any large organization engaged in the procurements or development of networks of heterogeneous computer systems.

500,713

PB86-111390 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Systems and Network Architecture Div.

Description of a Planned Federal Information Processing Standard for the Session Protocol.

Final rept.,
F. H. Nielsen, and J. F. Heafner. 1982, 7p
Pub. in Proceedings of COMPCOM 82, Digest of Papers Spring Conference on High Technology in the Information Industry, San Francisco, CA., February 22-25, 1982, p272-278.

Keywords: *Computer networks, *Standards, Specifications, Procurement, *Federal Information Processing Standards, *Open system interconnections, Session protocols.

The National Bureau of Standards has developed service and design specifications for internetwork, transport and session protocols for use in computer system and network procurements. These protocols reside in layers three, four, and five of the International Organization for Standardization's (ISO) Reference Model for Open Systems Interconnection. This paper describes the services and internal behavior of the session protocol. The session (and transport) protocol specifications were derived from the most recent developments within ISO on these protocols. Although specific features were selected based on the needs of U.S. Federal Government agencies, these needs are consistent with the needs of any large organization engaged in the procurement or development of networks of heterogeneous computer systems.

500,714

PB86-111408 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Systems and Network Architecture Div.

Description of a Planned Federal Information Processing Standard for File Transfer Protocol.

Final rept.,
F. H. Nielsen, and J. R. Moulton. 1982, 9p
Pub. in Proceedings of the INFOCOM 82, Las Vegas, NV., March 30-April 1, 1982, p139-147.

Keywords: *Computer networks, *Standards, Specifications, Procurement, *Federal Information Processing Standards, *Open system interconnections, *File transfer protocols.

The National Bureau of Standards has developed service and design specifications for transport, session, data presentation, and file transfer protocols for use in computer system and network procurements. These protocols reside in layers four, five, six and seven of the International Organization for Standardization's (ISO) Reference Model of Open Systems Interconnection. This paper describes the services and internal behavior of the file transfer protocol. The specification of the file transfer protocol, as well as specifications for the remainder of the aforementioned protocols, was derived from the most recent developments within ISO on this protocol. Specific features were selected based on the needs of the agencies of the Federal Government within the United States, but these needs are consistent with those of any large organization engaged in the procurement or development of networks of heterogeneous computer systems.

500,715

PB86-111887 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.

Microcomputers and the Writing of Programs.

Final rept.,
G. Lyon. 1982, 4p
Pub. in Proceedings of Trends and Applications 1982, Advances in Information Technology, Gaithersburg, MD., May 17, 1982, p65-68 1982.

Keywords: *Editing routines, Cost analysis, Microcomputers, Interactive programming.

Microcomputers are an inexpensive resource that will promote new ways of doing things, as opposed to doing older ways cheaper. An example illustrates how features of the attractive 'work sheet' programs can be extended to aid in program development via language-based constructors. Since microcomputer systems to support the heavy demands of these language-based methods are just becoming available, a brief examination is made of a suitable microcomputer configuration.

500,716

PB86-111895 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Systems and Software Technology Div.

Language-Based Editors/Interpreters.

Final rept.,
G. Lyon. Nov 82, 2p
Pub. in Proceedings of COMPSAC 82 IEEE Computer Society's International Computer Software and Applications Conference (6th), Chicago, IL., November 8-12, 1982, p611-612.

Keywords: *Editing, *Interpreters, Bibliographies, *Computer software, Programming languages.

One can argue that in many respects language-based editor-interpreters are a natural extension (into the area of programming staff) of the popular interactive 'spreadsheet' packages. A language-based system can take many forms - the list included here is a sampling of recent works.

500,717

PB86-112026 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Information Systems Engineering Div.

Framework for Logical-Level Changes Within Database Systems.

Final rept.,
G. H. Sockut. May 85, 19p
Pub. in Computer 18, n5 p9-17 May 85.

Keywords: Logic design, Reprints, *Data base management systems, *Data structures, *Data conversion, Front end processors.

The paper considers several types of changes that can take place within logical constructs of database systems, such as ordinary update, restructuring, data interchange, conversion, and support of an interface for one data model as a front end for a database management system of a different data model. A Data Model Processor (DMP), reviewed briefly herein, provides a unifying conceptual framework for defining and comparing types of changes such as those listed above, some of which may seem mutually unrelated at first glance. The paper describes practical uses of the changes.

500,718

PB86-112760 Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div.

Superconducting A/D Converter Using Latching Comparators.

Final rept.,
C. A. Hamilton, F. L. Lloyd, and R. L. Kautz. 1985, 3p
Pub. in IEEE (Institute of Electrical and Electronics Engineers) Transactions on Magnetics MAG-21, n2 p197-199 Mar 85.

Keywords: *Analog to digital converters, Josephson junctions, Superconductors, Reprints.

The paper describes the design and performance of a six-bit A/D converter using fast edge latching comparators. Simulations predicting conversion times of 100 ps and 100 MHz signal bandwidth are verified experimentally. The addition of a superconducting track/hold circuit in front of the A/D converter is expected to substantially improve the signal bandwidth.

500,719

PB86-113966 PC A05/MF A01
National Bureau of Standards, Gaithersburg, MD. Systems and Network Architecture Div.

NBS (National Bureau of Standards) Host to Front End Protocol,
C. M. Chernick. Aug 85, 93p NBSIR-85/3236

Keywords: *Computer networks, Interfaces, Protocols, Network flows, Multiplexing, *Front end processors, *Host computers, Communication networks, Offload, National Bureau of Standards.

'Front end' processors can be used to 'offload' communications processing from host computers. This paper describes a generic protocol (denoted HFEP) for host to (and from) front end communications processors. The HFEP, used in conjunction with additional, more user oriented protocols, such as ISO Transport or Virtual Terminal Protocol, can be used to offload these protocols. The NBS HFEP provides for a reliable, multiplexed, connection oriented services with a mechanism for process rendezvous. Primitives are defined for opening and closing connections, transferring data and determining the status of a connection. The HFEP uses underlying X.25 network technology (although other reliable, multiplexed and individually flow controlled network connection oriented technologies could be used.)

500,720

PB86-118700 CP T08
National Bureau of Standards, Gaithersburg, MD. Inst. for Computer Sciences and Technology.

ISO Connectionless Network Protocol - Implementation and Test System.

Software,
D. E. Rorrer, and M. A. Wallace. Oct 85, mag tape
NBS/SW/MT-86/001
Source tape is in the ASCII character set. This restricts preparation to 9 track, one-half inch tape only. Identify recording mode by specifying density only. Call NTIS Computer Products if you have questions.

Keywords: *Software, Computer programs, Standards, Tests, Magnetic tapes, Computer networks, L=C, H=DEC VAX-11/780, ISO standard.

The tape consists of programs which provide an implementation of the ISO Connectionless-Mode Network Service and a Test System which measures the conformance of an implementation to the ISO standard...Software Description: The program is written in the 'C' programming language for implementation on DEC VAX 11/780 computer using the EUINICE/VMS V5.7 operating system.

500,721

PB86-119187 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Inst. for Computer Sciences and Technology.

Role of Testing Tools and Techniques in the Procurement of Quality Software and Systems.

Final rept.,
J. C. Cherniavsky, W. R. Adrion, and M. A. Branstad. 1979, 5p
Pub. in Conference Record of the Asilomar Conference on Circuits, Systems and Computers (13th), Pacific Grove, CA., November 5-7, 1979, p309-313.

Keywords: *Computer systems programs, *Procurement, Quality control, Tests, Programming, Reprints, *Computer software, *Software tools.

The paper is oriented towards those quality control problems peculiar to the procurement of software. The authors discuss the deficiencies, and possible corrections, of several current methodologies. The authors propose a set of software management and development tools for software quality assurance which enables better contractor-developer communication during the development. The paper also includes a discussion of how sophisticated programming environments can play a central role in procured software development and a discussion of the associated research issues.

500,722

PB86-119260 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Inst. for Computer Sciences and Technology.

Processing Text Versus Editing and Formatting.

Final rept.,
C. P. Howerton. 1979, 2p
Pub. in CIPS Review 3, n6 p24-25 Dec 79.

Keywords: *Editing, Programming languages, Reprints, *Text processing, *Formats.

Field 9—ELECTRONICS AND ELECTRICAL ENGINEERING

Group 9B—Computers

The paper discusses various forms of text processing which are not classical and compares them to editing and formatting. Calls for creation of a super formatter which becomes a formal programming language in its optimal manifestation.

500,723

PB86-122850

Not available NTIS

National Bureau of Standards, Gaithersburg, MD. Systems Components Div.

Modular Expansion in a Class of Homogeneous Networks.

Final rept.,

A. Mink, and C. B. Silio. 1982, 5p

Sponsored by Association for Computing Machinery, New York.

Pub. in Proceedings of Computer Network Performance Symposium, College Park, MD., April 13-14, 1982, v11 n1 p95-100.

Keywords: *Computer networks, Modular structures, Expansion, Capacity, Performance, Queuing theory, *Computer architecture, Computer systems design.

The authors consider a special class of homogeneous computer network comprising several essentially identical but independent computing systems (ICSs) sharing a single resource. Of interest here are the effects of modularly expanding the network by adding ICSs. The authors use a previously presented approximate queuing network model to analyze modular expansion in this class of network. The performance measure used in this analysis is the mean cycle time, which is the mean time between successive requests for service by the same job at the CPU of an ICS. In this analysis the authors derive an intuitively satisfying mathematical relation between the addition of ICSs and the incremental increase in the service rate of the shared resource required to maintain the existing level of system performance.

500,724

PB86-122900

Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

Session Layer Protocols.

Final rept.,

F. H. Nielsen. 1982, 8p

Pub. in State of the Art Report Network Architectures, Series 10, n1 p191-198 1982.

Keywords: Standards, Proposals, Reprints, *Foreign technology, *Session protocols, *Computer networks, National Bureau of Standards.

The role and services of the Session layer in the ISO architecture is explained. A Session layer protocol proposed by the National Bureau of Standards is discussed. Also described is a proposal for a network interprocess communication protocol, which would reside in the Session layer.

500,725

PB86-123122

Not available NTIS

National Bureau of Standards, Gaithersburg, MD. Data Management and Programming Languages Div.

Developing a Programming Environment.

Final rept.,

M. V. Zelkowitz. 1981, 6p

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

Pub. in Proceedings of Annual Technical Symposium of the Washington, DC. Chapter of ACM (20th), Crisis in Computing: Innovation in a Constrained Environment, College Park, MD., June 18, 1981, p23-28.

Keywords: *Computer programming, Prototypes, Specifications, System analysis, *Translators, *Software engineering, *Software tools, *SNOBOL programming language, *High level languages.

There is a need to develop a prototype rapidly in order to be able to test systems specifications before a costly implementation is undertaken. The paper describes two research projects that aid in this effort. In one project, SNOBOL4 is used as a very high level executable design language in order to develop a rapid prototype of a language translator. In a second project, an intelligent data base is being designed to aid in developing PL/I programs. This PL/I system will have some of the characteristics of the earlier SNOBOL4 system. An eventual goal of this research is to later include a high level design language like SNOBOL4 to totally merge the two concepts into one system.

500,726

PB86-124088

Not available NTIS

National Bureau of Standards, Gaithersburg, MD. Systems and Network Architecture Div.

Protocol Standardization.

Final rept.,

L. J. Miller. 1980, 7p

Pub. in Proceedings of EASCON '80 Record IEEE (Institute of Electrical and Electronics Engineers) Electronics and Aerospace Systems Conventions, Arlington, VA., September 29-October 1, 1980, p507-513.

Keywords: *Standards, *Computer networks, *Open system interconnections, Distributed computer systems, Network analysis, Protocols.

The paper describes the seven layers of the Reference Model of Open Systems Interconnection which has been developed by the International Organization for Standardization, and indicates other areas of network protocol standardization activity within ANSI, ISO, and CCITT. The National Bureau of Standards' program in Computer Network Protocol Standards is then described. This program involves the design, implementation, impact study, evaluation, and standardization of a family of protocols considered necessary for the development of distributed networks within the Federal Government.

500,727

PB86-124799

Not available NTIS

National Bureau of Standards, Gaithersburg, MD. Systems and Network Architecture Div.

Data Transfer Protocol for Remote Database Access.

Final rept.,

P. S. C. Wang, and S. R. Kimbleton. 1980, 82p

Pub. in Proceedings of Trends and Applications: 1980 Computer Network Protocols, Gaithersburg, MD., May 29, 1980, p701-782.

Keywords: *Computer networks, *Data transfer protocols, Data bases, Access, Remote systems.

A Data Transfer Protocol (DTP) is a protocol for transferring data, in a meaning-preserving way, among different hosts of a computer network. The design of DTPs is separated into the following components: (1) specification of the services provided; (2) description of the internal structure of the protocol (in the form of descriptions of the individual entities of the DTP and the messages exchanged among these entities); and (3) identification of the required lower level support functions. The paper considers, in detail, the above three aspects of the design of a specific DTP.

500,728

PB86-124807

Not available NTIS

National Bureau of Standards, Gaithersburg, MD. Center for Computer Systems Engineering.

Network Access Technology: A Perspective.

Final rept.,

S. W. Watkins, and S. R. Kimbleton. 1978, 9p

Pub. in AFIPS (American Federation of Information Processing Societies), Conference Proceedings, Anaheim, CA., June 5-8, 1978, v47 p495-503.

Keywords: *Telecommunication, *Computer networks, Computer components, Evaluation, *Access methods, Support services.

Effective user access to network resources is inhibited by differences in command languages, operating systems functions, file naming conventions, and system idiosyncrasies. This has resulted in the gradual development of network access support aids which offload many access related problems from the user to a support system. The paper: (i) overviews the area of network access; (ii) identifies related research efforts; (iii) identifies some of the factors which make network access support difficult; and (iv) structures major access support components. Insights resulting from the current implementation of one of these components, expert assistance, are also presented.

500,729

PB86-124815

Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

Measurement of Control and Data Flow Complexity in Software Designs.

Final rept.,

M. H. Whitworth, and P. A. Szulewski. 1980, 9p

Pub. in Proceedings of COMPSAC 80 IEEE (Institute of Electrical and Electronics Engineers) Computer Society's International Computer Software and Applications (4th) Conference, Chicago, IL., October 27-31, 1980, p735-743.

Keywords: *Software engineering, *Data flow analysis, *Software quality control, *Computer systems design.

Progress in the areas of software development methodology and software quality measurement have lagged far behind the advances made in other computer-related fields. Most previous work in software quality assessment has addressed the quality of computer code. In the paper, the focus is shifted and the quality of software designs is emphasized. Two metrics of design complexity are proposed (complexity is often cited as having a negative impact upon software quality). By allowing software quality assessment techniques to be applied in the design phase of the development cycle, continuous evaluation of alternative designs is facilitated.

500,730

PB86-124849

Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

Lexical Synthesis Approach to User-Oriented Input Specification.

Final rept.,

C. Witzgall, and K. Hoffman. 1978, 8p

Pub. in Proceedings of Annual Technical Symposium on Tools for Improved Computing in the 80's (17th), Gaithersburg, MD., June 15, 1978, p178-185.

Keywords: Word organized storage, Decoding, Specifications, Words(Language), *Applications programs(Computers), Natural language, User needs.

Modern large-scale application programs often call for flexible natural-language type input capabilities. The paper presents a general and highly flexible 'lexical synthesis' approach to the lexical decoding problem based on systematic string recognition rather than delimiting rules. It has successfully been implemented in an operating general-purpose lexical synthesis package ULEX.

500,731

PB86-124948

Not available NTIS

National Bureau of Standards (NML), Gaithersburg, MD. Office of Standard Reference Data.

Status and Trends of Numeric Data Banks.

Final rept.,

J. Rumble. 1983, 5p

Sponsored by Polish Academy of Sciences, Warsaw. Inst. of Physical Chemistry.

Pub. in Proceedings of International CODATA Conference (8th) Data for Science and Technology, Jachranka, Poland, October 4-7, 1982, p188-192 1983.

Keywords: Numbers, Interfaces, Trends, *Data banks, *Scientific data, Machine translations, User needs, On-line systems.

The paper discusses the present-day status and trends of scientific numeric data banks. The main emphasis is on the user interfaces to data banks which provide the extra capability to computer-readable data which distinguishes them from the paper data banks.

500,732

PB86-126687

PC A05/MF A01

National Bureau of Standards, Gaithersburg, MD.

Benchmark Analysis of Database Architectures: A Case Study.

Final rept.,

S. B. Yao, A. R. Hevner, and D. R. Benigni. Oct 85,

100p NBS/SP-500/132

See also PB85-155794. Also available from Supt. of Docs as SN003-003-02684-1. Library of Congress catalog card no. 85-600599. Prepared in cooperation with Software Systems Technology, Inc., College Park, MD.

Keywords: Performance evaluation, Guidelines, Microcomputers, Minicomputers, *Data base management systems, *Data bases, *Benchmarks, Analysis, Computer architecture.

The purpose of this guideline is to present an application of the generalized performance analysis methodology for the benchmarking of database systems that was reported in NBS Special Publication 500-118. The principal objectives of this guide are to benchmark the performance of three distinct database system architectures: (1) a microcomputer database system; (2) a minicomputer database system; and (3) a database machine. This guide not only proves the viability of the benchmarking methodology in evaluating real systems, but it also provides comparable observations as to the capabilities of database systems based upon

different architectures. Together with NBS Special Publication 500-118, this report serves as a reference for the benchmarking of database systems by providing a complete description of the benchmarking framework and a detailed application showing how to implement it.

500,733

PB86-126745 PC A04/MF A01
National Bureau of Standards, Gaithersburg, MD.
Center for Programming Science and Technology.
Software Maintenance Management.

Final rept.,
J. A. McCall, M. A. Herdon, and W. M. Osborne. Oct 85, 71p NBS/SP-500/129

Also available from Supt. of Docs as SN003-003-02681-6. Library of Congress catalog card no. 85-600596. Prepared in cooperation with Science Applications, Inc., La Jolla, CA.

Keywords: *Computer software, *Data processing, Management, *Computer software maintenance, *Computer software management, Software quality, Software tools, Life cycle costs, Federal agencies.

The report presents an overview of the various aspects of software maintenance, and provides an in-depth analysis of the associated problems, giving particular attention to the most pressing ones. It identifies tools, techniques, and procedures which aid in reducing these problems. This report also provides detailed guidance for managing software maintenance as a separate organizational entity. It also provides assistance needed to develop and employ improved maintenance practices and procedures, that result in reduced software costs and which help to insure that quality software is developed for and by the Federal ADP community.

500,734

PB86-128212 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Data Management and Programming Languages Div.
Data Models: Keys to Understanding Data Base Management Systems.

Final rept.,
D. R. Deutsch, and J. M. Draper. 1984, 21p
Pub. in *Advances in Data Base Management 2*, Chapter 1, p1-21 1984.

Keywords: Selection, Standardization, Computer software, *Data base management systems, *Data structures, Relational data bases, Hierarchical data bases, Network data bases.

A data model describes the essential characteristics, including the logical data structures and operations, of an approach to data base management. This chapter demonstrates the pedagogical use of the data model concept by applying it to the relational, network, and hierarchical data models. After these descriptions the role of data models in the selection and standardization of data base management systems is examined.

500,735

PB86-128782 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD.

Tomographic Image Reconstruction from Limited Projections Using Iterative Revisions in Image and Transform Spaces.

Final rept.,
T. Sato, S. J. Norton, M. Linzer, O. Ikeda, and M. Hiram. 1981, 5p
Pub. in *Applied Optics* 20, n3 p395-399, 1 Feb 81.

Keywords: Fourier transformations, Ultrasonic radiation, Iterations, Reprints, *Image reconstruction, Tomography.

An iterative technique is proposed for improving the quality of reconstructions from projections when the number of projections is small, or the angular range of projections is limited. The technique consists of transforming repeatedly between image and transform spaces and applying a priori object information at each iteration. Information which is often known a priori and may be used in this manner are the outer boundaries of the object and the limits on the range of variation of the physical parameters of interest. This process of forcing the image to conform to a priori object data can help to reduce artifacts arising from incomplete or limited data available in the Fourier transform plane. The results of computer simulations show clearly the effectiveness of the proposed approach.

500,736

PB86-128816 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Systems and Network Architecture Div.
Analysis of Link Level Protocols for Error Prone Links.

Final rept.,
L. J. Miller. 1981, 6p
Pub. in *Proceedings of Data Communications Symposium* (7th), Mexico City, Mexico, October 27-29, 1981, *Comput. Commun. Rev.* 11, n4 p130-135 Oct 81.

Keywords: *Data links, *Duplexers, Errors, *Computer communications, Protocols, Throughput, Computer performance evaluation, Packet switching.

The paper analyzes the maximum throughput across a full duplex link, under three link level protocols. The three protocols all assume cumulative acknowledgements, but the sender's retransmission policy and the destination's policy on retaining correctly received packets which arrive before an expected retransmission differ. The results quantify the throughput advantages in retaining all correctly received packets, for the two different retransmission policies. A retention policy on the part of the destination is most advantageous when the link is quite error-prone.

500,737

PB86-129012 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Systems and Software Technology Div.
Summary of the NBS (National Bureau of Standards) Programming Environment Workshop.

Final rept.,
M. A. Branstad. 1981, 5p
Pub. in *Proceedings of Annual Technical Symposium* (20th) on Crisis in Computing: Innovation in a Constrained Environment, College Park, MD., June 18, 1981, p39-43.

Keywords: *Computer programming, Productivity, Meetings, *Software engineering, *Software tools, *Software quality control, Workshops, National Bureau of Standards.

In May of 1980 NBS hosted a workshop to assess the state of the art in programming environment technology and to determine the key questions and issues that must be addressed to use these techniques to improve software quality and productivity within the Federal Government. This paper summarizes the results of the workshop.

500,738

PB86-129749 PC A03/MF A01
National Bureau of Standards, Gaithersburg, MD. Inst. for Computer Sciences and Technology.

Characteristics and Functions of Software Engineering Environments.

Research rept. 1 Oct 84-19 Sep 85,
R. C. Houghton, and D. R. Wallace. Sep 85, 45p
NBSIR-85/3250
Prepared in cooperation with Duke Univ., Durham, NC.

Keywords: Life cycles, *Software quality control, *Software engineering, *Software tools, Computer software maintenance.

As part of the program to provide information to Federal agencies on software tools for improving quality and productivity in software development and maintenance, data was collected on software engineering environments. Software engineering environments surround their users with software tools necessary for systematic development and maintenance of software. The purpose of this report is to characterize software engineering environments by type and by their relationship to the software life cycle and by their capabilities, limitations, primary users, and levels of support. This report provides examples of existing software engineering environments that are available commercially or in research laboratories with the features and characteristics they provide.

500,739

PB86-129954 PC A10/MF A01
National Bureau of Standards, Gaithersburg, MD. Center for Programming Science and Technology.

Technology Assessment: Methods for Measuring the Level of Computer Security.

Final rept. 1980-81,
W. Neugent, J. Gilligan, L. Hoffman, and Z. G. Ruthberg. c1985, 208p NBS/SP-500/133
See also FIPS PUB-102. Also available from Supt. of Docs as SN003-003-02686-7. Library of Congress

catalog card no. 85-600600. Prepared in cooperation with System Development Corp., McLean, VA., and George Washington Univ., Washington, DC.

Keywords: Evaluation, Auditing, Guidelines, Risk, Verifying, *Computer security, *Federal information processing standards, Certification, Analysis.

The document is a companion to FIPS PUB 102, 'Guideline for Computer Security Certification and Accreditation.' Since a security certification depends upon a technical security evaluation, this document is meant to provide information on and insight about twenty-five evaluation methods in common use today in the security, EDP audit, and risk analysis communities.

500,740

PB86-132107 PC A04/MF A01
National Bureau of Standards, Gaithersburg, MD. Center for Programming Science and Technology.
Guide for Selecting Microcomputer Data Management Software.

Final rept.,
C. L. Sheppard. Oct 85, 69p NBS/SP-500/131
Also available from Supt. of Docs as SN003-003-02682-4. Library of Congress catalog card no. 85-600598.

Keywords: *Microcomputers, Bench marks, Data processing, Selection, *Computer software, *Applications programs(Computers), File management systems, Data bases, User manuals(Computer programs).

No abstract available.

500,741

PB86-132693 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Automated Production Technology Div.

Summary Assessment of the Symposium on the Role of Language in Problem Solving.

Final rept.,
J. C. Boudreaux. 1985, 8p
Pub. in *Role of Language in Problem Solving I*, p341-348 1985.

Keywords: *Meetings, *Problem solving, *Programming languages, Reprints.

The paper summarizes the significant results of the Symposium on the Role of Language in Problem Solving, and states a series of open questions in the design of programming languages and programming environments.

500,742

PB86-132701 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Automated Production Technology Div.

Problem Solving and the Evolution of Programming Languages.

Final rept.,
J. C. Boudreaux. 1985, 24p
Pub. in *Role of Language in Problem Solving I*, p103-126 1985.

Keywords: *Programming languages, Evolution(Development), Problem solving, Automation, Transformational grammars, Cognition, Computation, Design, Reprints, *Foreign technology, *High level languages, User needs.

Backus has observed that von Neumann programming languages are fat and weak. Though there are current efforts to provide alternate models of computation, an examination of the genealogy of programming languages suggests that it is unlikely that the issues now facing programming language designers will be resolved by the simple expedient of replacing one model with another. What such an examination does suggest is that each succeeding generation transfers new and more difficult cognitive functions from the programmer to the computer. If this is correct, then the author can predict that the next generation will come about not by some revolutionary advance in computer technology, but by the successful automation of higher-order cognitive functions which now require human attention. One ideal solution would be a cluster of programming languages that are expressive enough to reflect as nearly as possible the user's own cognitive framework, i.e., the structured world of abstract objects which define the user's application domain, together with the set of transformation rules on that domain which permit the user to create and/or modify those objects.

Field 9—ELECTRONICS AND ELECTRICAL ENGINEERING

Group 9B—Computers

The paper examines existing programming languages and then shows how ideal programming languages could be realized in practice.

500,743
PB86-133469 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Automated Production Technology Div.
Solid Modeling, Aspect Graphs, and Robot Vision.
Final rept.,
G. M. Castore. 1984, 15p
Pub. in Solid Modeling by Computers: From Theory to Applications, p277-292 1984.

Keywords: *Pattern recognition, *Computer vision, *Robot vision, PADL-2 system, Geometric modelling.

At the National Bureau of Standards, a method is being developed for transferring sufficient information directly from the solid modeling system to the robot vision system to enable the robot to recognize a part. The information is encoded in the form of a graph, called an aspect graph, together with functions associated to each vertex of the graph. Aspect graphs were developed by J.J. Koenderink of the State University of Utrecht in the Netherlands, as part of an attempt to understand how shape information is represented by the human vision system. Currently the method is being developed for parts designed on the PADL-2 system. In particular, it does not yet handle contoured surfaces. Extensions to deal with contoured surfaces appear to be feasible and are mentioned briefly.

500,744
PB86-133618 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Scientific Computing Div.
Operating a Local Area Network.
Final rept.,
R. J. Crosson. 1983, 5p
Pub. in Proceedings of Computer Networking Symposium, Silver Spring, MD., December 3, 1983, p73-77.

Keywords: *Computer networks, Standards, Operations, *Ethernet computer network, *NBSNET computer network, *Local area network, Computer systems design, Protocols, Operating systems(Computers), User needs.

NBSNET is a baseband Ethernet-like network at the National Bureau of Standards serving over 400 nodes. Connected devices communicate with the network using three types of protocols - one for terminals, and two for computers. The protocols contain flexibility to accommodate the unique facilities of the user's equipment. The lessons learned from the NBSNET experience are that capabilities for coping with user's equipment and for diagnosing problems encountered in the network's operation must be integral parts of the network's design. Also, the lack of standards increases the amount and level of support required.

500,745
PB86-138112 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Systems Components Div.
Institute for Computer Sciences and Technology at the National Bureau of Standards (NBS/ICST) Optical Digital Data Disk (OD sup 3) Standardization Activities.
Final rept.,
J. B. Freedman. 1984, 3p
Pub. in Proceedings of the Society of Photo-Optical Instrumentation Engineers: Applications of Optical Digital Data Disk Storage Systems, Brussels, Belgium, June 25-28, 1984, v490 p77-79.

Keywords: *Computer storage devices, *Standardization, *Optical disks, Disk recording systems, National Bureau of Standards.

The paper describes the optical digital disk (OD/sup 3/) standardization activities including the NBS-sponsored Federal Council on Computer Storage Standards and Technology (FCCSSAT); the National Bureau of Standards/National Security Agency Workshop on standardization issues for OD/sup 3/ technology; and the NBS/ICST participation in the voluntary OD/sup 3/ standards process. All of the NBS/ICST activities provide a forum for discussion among current and potential OD/sup 3/ users and suppliers, regarding the prospects for OD/sup 3/ data interchange standardization.

500,746
PB86-138161 Not available NTIS

National Bureau of Standards, Gaithersburg, MD. Data Management and Programming Languages Div.
Procedure Language Access to Proposed American National Standard Database Management Systems.
Final rept.,
L. J. Gallagher. 1984, 12p
Pub. in Comput. Networks 8, n1 p31-42 Feb 84.

Keywords: *Procedure oriented languages, Standards, Specifications, Reprints, *Data base management systems, *Application programs(Computers), *Relational data bases, *Open system interconnections, *Access methods, Distributed processing.

Network and relational database standards are under development by technical committee X3H2 of the American National Standards Institute. This paper is an overview of the procedure language interface to these proposed standards. It introduces the basic structures and operations of each data model, focuses on the procedure language interface as a facility for database access from external languages, and discusses various alternatives for use of the database language standard with existing standard programming languages. The paper contains example application programs of each access alternative and concludes with a discussion of basic requirements for application of the standard specifications to distributed database processing in an open systems environment.

500,747
PB86-138195 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Data Management and Programming Languages Div.
Distributed Database Management Systems: An Architectural Perspective.
Final rept.,
V. D. Gligor, and E. N. Fong. 1983, 22p
Pub. in Jnl. of Telecommunications Networks 2, n3 p249-270 1983.

Keywords: Global communication, Data links, Heterogeneity, Telecommunication, Reprints, *Data base management systems, *Distributed processing, Computer systems design, Remote systems, Architecture(Computers), Communication networks.

Several distributed Database Management Systems which have been developed in the U.S., Europe, and Japan are reviewed in the paper. Most of the systems discussed are the result of various experimental projects. The basis for the review is provided by an architectural model which includes a set of necessary features for the interconnection of remote, heterogeneous systems. These features refer to the user-visible layers of a general, distributed DBMS architecture, and include those of the Global Data Management layer and of the Distributed Transaction Management layer.

500,748
PB86-138385 Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div.
Pattern Recognition Using Incoherent OTF (Optical Transfer Function) Synthesis and Edge Enhancement.
Final rept.,
Y. Katzir, M. Young, and I. Glaser. Mar 85, 5p
Pub. in Applied Optics 24, n6 p863-867, 15 Mar 85.

Keywords: *Pattern recognition, Character recognition, Holography, Reprints, Optical correlators, Optical transfer functions, Optical processing, Robot vision, Image enhancement.

The paper describes a system for pattern recognition using an incoherent-optical correlator. The system uses optical transfer function synthesis to perform correlations with an edge-enhanced image of the object or pattern being sought. The resulting correlations are free of bias and show good discrimination between objects. In addition, the difficult or time-consuming computations are performed before the operation of the system; this reduces the amount of postprocessing by computer and should allow real-time operation at video rates.

500,749
PB86-138500 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Systems and Software Technology Div.

Online Help Systems - A Conspectus.
Final rept.,
R. C. Houghton. 1984, 8p
Pub. in Communications of the Association for Computing Machinery 27, n2 p126-133 1984.

Keywords: *Assistance, Human factors engineering, Reprints, *On line systems, *Help systems, Man machine systems.

Users of computer systems have become accustomed to the convenience of on-line help systems and, as a result, require the availability of help systems on computers they purchase. There are many types of assistance that can be provided by help systems and there are many issues to be considered by the developers of such systems. The types of assistance include command assistance, help assistance, error assistance, on-line tutors and on-line documentation. Development issues include the quality and style of the assistance, query-in depth, contextual assistance, use of natural language, use of simulation, consistency, and contextual mode switching. Experiments with help systems underline many of these issues.

500,750
PB86-138997 PC A11/MF A01
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.
Device Independent Graphics Kernel.
W. W. Jones, and A. B. Fadell. Oct 85, 245p NBSIR-85/3235

Keywords: *Computer graphics, *Display devices, Interfaces, *Computer program transferability, *Machine-independent programs, Input output devices, User needs.

The paper describes an interface for programs which allows one to write graphics primitives to several devices without regard for the type of device. The most salient features are that it has low overhead, is transportable and can be expanded as the nature of the input/output devices changes. A conscious effort has been made to include all normal graphics primitives together with the most useful high level routines without compromising the use of special features of custom display units.

500,751
PB86-140258 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Systems Components Div.
Supercomputers.
Final rept.,
J. P. Riganati, and P. Schneck. 1984, 17p
Pub. in Computer 17, n10 p97-113 Oct 84.

Keywords: *Computers, United States, Japan, Trends, Reprints, *Supercomputers, Taxonomy.

The overview describes the development and current status of supercomputers. It considers fundamental and conjectured limitations, characterizes existing systems being produced in the U.S. and Japan and discusses the difficulties inherent in performance measurement and in creation of a suitable taxonomy. Current trends and future possibilities are briefly reviewed.

500,752
PB86-142494 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Center for Computer Systems Engineering.
National Bureau of Standards Computer Based Message Systems Standards Efforts: A Status Report.
Final rept.,
S. W. Watkins. 1982, 6p
Pub. in Proceedings of International Conference Communications (6th), Pathways to the Information Society, London, England, September 7-10, 1982, p289-294.

Keywords: *Computers, *Standards, Reprints, *Message systems, National Bureau of Standards.

A major component of the National Bureau of Standards (NBS) Computer Based Office Systems program is devoted to the area of Computer Based Message Systems (CBMSs). A CBMS allows communication among entities using computers. The computer's role in this messaging process is threefold: assistance to the user for message creation, assistance to the user for message reading and storage, and mediation of the actual communications. This paper provides an overview of

the NBS program for CBMS standards, discusses the technical specifications of the first proposed standard out of this program which is for message format for CBMS, and introduces NBS work on a message transfer protocol.

9C. Electrical and Electronic Engineering

500,753

PATENT-4 520 320 Not available NTIS
Department of Commerce, Washington, DC.
Synchronous Phase Marker and Amplitude Detector.

Patent,
J. E. Potzick, and B. Robertson. Filed 22 Feb 84, patented 28 May 85, 30p PB85-211621, PAT-APPL-6-571 288
This Government-owned invention available for U.S. licensing and, possibly, for foreign licensing. Copy of patent available Commissioner of Patents, Washington, DC 20231 \$1.00.

Keywords: *Phase meters, Phase shift, Amplitude, PAT-CL-328-133.

Disclosed is an electronic circuit for determining the phase difference between an input signal and a reference signal where both signals are of the same frequency. Furthermore, the circuit provides an amplitude output indicative of the input signal even when that signal is obscured by noise.

500,754

PB85-187540 PC A03/MF A01
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Electronics and Electrical Engineering. **Center for Electronics and Electrical Engineering Technical Progress Bulletin Covering Center Programs, April-June 1984 with 1984 CEEE (Center for Electronics and Electrical Engineering) Events Calendar,** J. F. Mayo-Wells. Jul 84, 26p NBSIR-84/2877/2 See also PB84-222785.

Keywords: *Electrical engineering, *Electronics, *Metrology, Semiconductors(Materials), Signals, Electromagnetic interference, Antennas, Standard reference materials.

This is the seventh issue of a quarterly abstract journal covering the work of the National Bureau of Standards Center for Electronics and Electrical Engineering. This issue of the Center for Electronics and Electrical Engineering Technical Progress Bulletin covers the second quarter of calendar year 1984. Abstracts are provided by technical area for both published papers and papers approved by NBS for publication.

500,755

PB85-191393 PC A02/MF A01
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Electronics and Electrical Engineering. **Center for Electronics and Electrical Engineering Technical Progress Bulletin Covering Center Programs, July - September 1984 with 1985 CEEE Events Calendar,** J. F. Mayo-Wells. Dec 84, 25p NBSIR-84/2877-3 See also PB84-222785.

Keywords: *Electrical engineering, *Electronics, *Metrology, Semiconductors(Materials), Signals, Antennas, Electromagnetic interference, Standard reference materials.

This is the eighth issue of a quarterly abstract journal covering the work of the National Bureau of Standards Center for Electronics and Electrical Engineering. This issue of the Center for Electronics and Electrical Engineering Technical Progress Bulletin covers the third quarter of calendar year 1984. Abstracts are provided by technical area for both published papers and papers approved by NBS for publication.

500,756

PB86-113057 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD.

Informal Survey of Federal Government Microelectronics Processing Facilities.

Final rept.,
M. C. Peckerar, and K. F. Galloway. 1981, 7p
Sponsored by Naval Research Lab., Washington, DC. Pub. in Proceedings of University, Government, Industry, Microelectronics Symposium, Starkville, MI., May 26-28, 1981, p3.24-3.30.

Keywords: *Microelectronics, National government, Laboratories, Processing, Facilities, Survey, Universities, Statistical data, Reprints.

A number of microelectronics processing facilities associated with Federal Government laboratories or installations have been surveyed by telephone. Data is presented on available equipment, general missions, and possibilities for university personnel to interact with these facilities.

500,757

PB86-129053 Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Fields Div.
Broadband Noise Source Applications.

Final rept.,
W. C. Daywitt. 1985, 2p
Pub. in Proceedings of Institute of Electrical and Electronics Engineers 1985 Instrumentation and Measurement Technology Conference, Tampa, FL., March 20-22, 1985, p165-166.

Keywords: *Thermal noise, *Standards, Measurement, Telecommunication, Communication satellites, *Noise temperature, Spacecraft communications.

Accurate noise characterization of amplifiers and communication systems requires the use of thermal noise standards. The note is a brief review of the use of such standards as a basis for the measurement of effective input noise temperature and the G/T of a satellite earth terminal receiving system.

500,758

PB86-132032 PC A06/MF A01
National Bureau of Standards, Gaithersburg, MD. **Calibration of Test Systems for Measuring Power Losses of Transformers.**
Final rept.,
O. Petersons, and S. P. Mehta. Sep 85, 108p NBS/TN-1204
Also available from Supt. of Docs as SN003-003-02677-8. Prepared in cooperation with ASEA Electric, Inc., Waukesha, WI.

Keywords: *Calibrating, *Test equipment, Power loss, Measurement, Power transformers.

A calibration system for accuracy verification and alignment of test systems for measuring transformer losses is described. Methodologies are presented for assessing measurement uncertainties and for evaluating overall accuracy of test systems. Procedures are suggested for continuing maintenance and calibration of standard instruments and test systems to ensure traceable measurements.

500,759

PB86-134871 PC A09/MF A01
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Electronics and Electrical Engineering. **Proceedings of Seminar on Digital Methods in Waveform Metrology Held at Gaithersburg, Maryland on October 18-19, 1983,** B. A. Bell. Oct 85, 177p NBS/SP-707
See also PB86-134889 through PB86-134962. Also available from Supt. of Docs as SN003-003-02694-8. Library of Congress catalog card no. 85-600591.

Keywords: *Metrology, *Meetings, *Waveforms, Synthesis, Sampling, Data converters, Electronic test equipment, Standards, Calibrating.

The special publication contains complete papers on the subjects presented at the seminar, providing more of the technical details. For the sessions on Precision Waveform Synthesis, Precision Waveform Sampling, and Data Converter Characterization, six formal papers are given describing the hardware and software techniques used for developing NBS laboratory standards and apparatus for testing ac sources and voltmeters, phase angle meters, transient waveform recorders, wideband wattmeters, and digital-to-analog and analog-to-digital converters. For the informal session on Instrumentation Metrology, three subsequent papers have been written for publication which are included for completeness in the Appendices.

500,760

PB86-134897
(Order as PB86-134871, PC A09/MF A01)
National Bureau of Standards (NEL), Gaithersburg, MD. Electrosystems Div.
Phase Angle Standards and Calibration Methods, R. S. Turgel. Oct 85, 15p
Included in Proceedings of Seminar on Digital Methods in Waveform Metrology, p15-29 Oct 83.

Keywords: *Phase angle, Standards, Calibrating, Measurement.

Topics include measurement principles, source or error, phase-angle calibration standards, NBS phase-angle calibration standard, other digital phase standards, and calibration strategies.

500,761

PB86-134905
(Order as PB86-134871, PC A09/MF A01)
National Bureau of Standards (NEL), Gaithersburg, MD. Electrosystems Div.
Characterization of Waveform Recorders, D. R. Flach. Oct 85, 24p
Included in Proceedings of Seminar on Digital Methods in Waveform Metrology, p31-54 Oct 83.

Keywords: Tests, Recording instruments, *Waveform recorders.

Although transient waveform recorders have been in use for more than 15 years, no commonly accepted test procedures were in use for these instruments, particularly for the evaluation of errors associated with dynamic input signals. The tests described are essentially those in which the final output of the test is the result of digital signal processing on the waveform recorder's digital output.

500,762

PB86-134913
(Order as PB86-134871, PC A09/MF A01)
National Bureau of Standards (NEL), Gaithersburg, MD. Electrosystems Div.
Dual-Channel Sampling Systems, G. N. Stenbakken. Oct 85, 19p
Included in Proceedings of Seminar on Digital Methods in Waveform Metrology, p55-73 Oct 83.

Keywords: *Electronic test equipment, *Sampling, Electric power, Measurement.

The paper will concentrate mainly on the application of dual-channel sampling techniques to the measurement of electrical power and, to a lesser extent, on the application to electrical phase angle measurements. Theoretical relationships are developed for describing these sampling measurements and their associated errors. The procedures that can be used to calibrate such dual-channel instruments for these applications will be described as well.

500,763

PB86-134921
(Order as PB86-134871, PC A09/MF A01)
National Bureau of Standards (NEL), Gaithersburg, MD. Electrosystems Div.
Data Converter Test Methods, T. M. Souders. Oct 85, 11p
Included in Proceedings of Seminar on Digital Methods in Waveform Metrology, p75-85 Oct 83.

Keywords: Calibrating, *Automatic test equipment.

A method of verifying the performance of automatic test equipment (ATE) in its normal operating environmental and configuration is presented as the best approach to achieving an overall system calibration. The method consists of the transport of well-characterized signal sources to the ATE station and the application of these electrical stimuli directly to a well-defined electrical interface on the test station. Data is presented on typical accuracies that have been obtained on limited parameters and ranges during the testing process, using calibrated commercial equipment.

500,764

PB86-134939
(Order as PB86-134871, PC A09/MF A01)
National Bureau of Standards (NEL), Gaithersburg, MD. Electrosystems Div.

Field 9—ELECTRONICS AND ELECTRICAL ENGINEERING

Group 9C—Electrical and Electronic Engineering

Settling Time Measurements,

H. K. Schoenwetter. Oct 85, 23p

Included in Proceedings of Seminar on Digital Methods in Waveform Metrology, p87-109 Oct 83.

Keywords: *Data converters, Tests, Instruments.

A/D and D/A converters are presently being produced in a vast array of types and models, exhibiting a wide range of design approaches, operating speeds, and accuracies for a wide variety of applications. As might be expected, an equally large number of test methods has been developed, with each addressing the measurement of some specific characteristics of one or more of these types or models. It is the intent of this tutorial to review the more useful, and hence more widely used, test methods pertinent to the characterization of data converters for use in measurement or control instrumentation applications.

500,765

PB86-134947

(Order as PB86-134871, PC A09/MF A01)
National Bureau of Standards (NEL), Gaithersburg, MD. Electrosystems Div.

Automatic AC/DC Thermal Voltage Converter and AC Voltage Calibration System,

K. J. Lentner, D. R. Flach, and B. A. Bell. Oct 85, 27p

Included in Proceedings of Seminar on Digital Methods in Waveform Metrology, pA1-A27 Oct 83.

Keywords: *Electrical measurement, Settling time, Microseconds.

Methods of measuring device settling times (STs) from 5 microseconds to less than 20 ns with corresponding accuracies of 1 ppm and 0.1% are described. Most of these methods are thought to represent state-of-the-art techniques, developed at NBS and in industry. Some of the ST measurement methods discussed are described in a March, 1983 paper. Only a brief review of these methods will be given, showing only the salient features. Some of the NBS work has been concerned with measuring thermally induced transients and offsets in devices under test (DUTs). Methods of measuring these effects with ST measuring circuits are described.

500,766

PB86-134954

(Order as PB86-134871, PC A09/MF A01)
National Bureau of Standards (NEL), Gaithersburg, MD. Electrosystems Div.

Gallium Arsenide (GaAs)-Based Photoconductive Switches for Pulse Generation and Sampling Applications in the Nanosecond Regime,

B. A. Bell, A. G. Perrey, and R. A. Sandler. Oct 85, 22p

Prepared in cooperation with ITT Gallium Arsenide Technology Center, Roanoke, VA.
Included in Proceedings of Seminar on Digital Methods in Waveform Metrology, pA28-A49 Oct 83.

Keywords: *Electric potential, Calibrating, Voltage converters, Voltage, Automatic test equipment.

An automatic ac/dc difference calibration system is described which uses direct measurement of thermoelement emfs. In addition to ac/dc difference testing, the system can be used to measure some important characteristics or thermoelements, as well as to calibrate ac voltage calibrators and precision voltmeters. The system operates over a frequency range from 20 Hz to 100 kHz, covering the voltage range from 0.5 V to 1 kV. For all voltages the total measurement uncertainties expected (including the uncertainty of the specific reference thermal converters used) were 50 parts per million (ppm) at frequencies from 20 Hz to 20 kHz, inclusive, and 100 ppm at higher frequencies up to 100 kHz.

500,767

PB86-142783

Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Electrosystems Div.

Emerging New Requirements for Electric Power and Energy Measurements.

Final rept.,

J. D. Ramboz, and O. Petersons. 1985, 10p

Pub. in Proceedings of the National Conference of Standards Laboratories Workshop and Symposium (1985), Boulder, Colorado, July 15-18, 1985, p3-12.

Keywords: *Electric measuring instruments, *Electric energy meters, Calibrating, Measuring instruments,

Precision, Measurements, Electric power meters, Watt hour meters.

Advances in electronic instrumentation technology have brought greater stability and precision to transducers that are utilized for measuring electric power and energy. An advantage of instruments based on electronic transducers is that they can be readily adapted to the measurement of other quantities such as current, voltage, reactive and apparent power, power factor, demand, time-of-day readings, etc. The calibration accuracies requested from NBS for power and energy measurements have increased at least fivefold (uncertainty reduction from $\pm 0.05\%$ to $\pm 0.01\%$) within the past several years. Calibrations for different quantities and values are being requested. These changing calibration requirements and the response of NBS to meet the requests of its calibration clientele are discussed.

500,768

PB86-142809

Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Fields Div.

Influence of Electromagnetic Interference on Electronic Devices.

Final rept.,

F. X. Ries, and C. K. S. Miller. 1981, 11p

Pub. in Bulletin OIML No. 85, p1-11 Dec 81.

Keywords: *Electromagnetic interference, *Electric devices, Electromagnetic radiation, Reprints.

The paper is intended to give the legal metrology weights and measures community an elementary understanding of the electromagnetic interference (EMI) problem associated with electronic devices. The approach followed here will be to first present a brief understanding of what electromagnetic (EM) waves are and the complexities involved in the understanding of their associated parameters. Following this is a discussion of the electromagnetic spectrum and its general pervasiveness and the effects changing technologies have had on electronic devices over the past forty years. A brief outline of the different types of testing methods and facilities will be presented.

500,769

PB86-143757

Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Electrosystems Div.

Power Calibration Standard Based on Digitally Synthesized Sinewaves.

Final rept.,

N. M. Oldham. Nov 85, 5p

Pub. in IEEE Transactions on Power Apparatus and Systems PAS-104, n11 p3117-3121 Nov 85.

Keywords: *Digital to analog converters, Inverters, Phase angle, Measurements, Reprints, *Calibration, *Calibration standards, Sine waves.

The unit of electric power at 60 Hz is often derived using impedance bridge techniques in which the alternating voltage is referred to the direct voltage standard through a thermal converter. An alternative calibration technique is described in which the ac to dc transfer is made through digital-to-analog converters (DACs) in the form of a dual-channel digital sinewave generator. The power is calculated from measurements of voltage, current, and phase angle, all of which rely on the accuracy of the digital generator and ultimately on the accuracy of the DACs.

9E. Subsystems

500,770

PB85-191419

PC A03/MF A01
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Fields Div.

Theory of Mutual Impedances and Multiple Reflections in an N-Element Array Environment.

Technical note,

L. A. Muth. Feb 85, 36p NBS-TN-1078

Also available from Supt. of Docs as SN003-003-02632-8.

Keywords: *Antenna arrays, Impedance, Theories, Reflection.

A general theoretical approach is formulated to describe the complex electromagnetic environment of an

N-element array. The theory reveals the element-to-element interactions and multiple reflections within the array. From the formulation, it is found that the interaction between an excited element and an open-circuited element can be viewed as the sum of terms describing all possible signal paths within the array environment which start from the radiating element and terminate on the element under observation. Within all paths except the most direct one, multiple reflections between subgroups of elements take place. The resulting solution is highly structured and recursive and is discussed in detail in the text. Illustrative examples are provided to facilitate understanding of these ideas.

500,771

PB85-197622

Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

Temperature Dependence of Transient Electron Radiation Upset in TTL NAND Gates.

Final rept.,

T. Leedy, G. McLane, and C. Guenzler. 1981, 9p

Sponsored by Defense Nuclear Agency, Washington, DC.

Pub. in Proceedings on IEEE (Institute of Electrical Electronics Engineers) Annual Conference on Nuclear and Space Radiation Effects, Seattle, WA., July 21-24, 1981, IEEE Transactions on Nuclear Science 28, n6 p4597-4605 Dec 81.

Keywords: *Integrated circuits, Radiation effects, Electron irradiation, Logic circuits, Gates(Circuits), Transistor transistor logic.

The temperature dependence of transient upset caused by a 40-MeV electron flux was investigated for junction-isolated gold-doped and nongold-doped TTL NAND gate devices in the temperature range from 20 to 125C. Data for five devices are presented.

500,772

PB85-202760

Not available NTIS

National Bureau of Standards (NEL), Gaithersburg, MD. Center for Electronics and Electrical Engineering.

Materials Measurements: Present Abilities and Future Needs.

Final rept.,

R. I. Scace. Mar 85, 4p

Pub. in Solid State Technology 28, n3 p155-158 Mar 85.

Keywords: *Integrated circuits, *Standards, Quality control, Measurement, Semiconductors(Materials), Processing, Reprints, Very large scale integration.

Standard measurement methods and specifications for the semiconductor industry are reviewed and discussed with emphasis on applications to VLSI processes. The standards development process is an excellent way for material producers and users to develop good working relations and to solve their shared measurement problems; this process is described in some detail. Because the semiconductor industry is an international one, serious efforts have been made for a number of years to rationalize the technical differences between test method standards in Europe and the U.S. with considerable success. The present state of such cooperative activity with Japan, which has a more recent origin, is also reported.

500,773

PB85-224475

PC A05/MF A01
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Fields Div.

Out-of-Band Response of Reflector Antennas,

D. A. Hill. Apr 85, 76p NBSIR-85/3021

Sponsored by Defense Nuclear Agency, Washington, DC.

Keywords: *Antennas, Performance evaluation, Applications of mathematics, Responses, Parabolic antennas, Out of band response.

The response of reflector antennas to out-of-band frequencies has been analyzed using physical optics. A simple approximate expression has been obtained for the effective aperture, and the expression yields both the receiving pattern and the frequency dependence of the on-axis gain. The theory has been compared with published out-of-band measurements, and the pattern agreement is good, but the measured gain falls below the theory. The discrepancy is caused by mismatch loss in the coax-to-waveguide adapter, and the mismatch loss has been analyzed theoretically. The basic physical optics model for symmetrical reflectors has been extended to include offset and dual reflec-

tors, reflector surface roughness, and transient excitation.

500,774
PB85-226892 PC A02/MF A01
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Fields Div.
Bibliography of the NBS (National Bureau of Standards) Electromagnetic Fields Division Publications, January 1982 through December 1983, K. A. Gibson, and C. K. S. Miller. Apr 85, 20p NBSIR-85/3022
See also PB83-119776.

Keywords: *Antennas, *Electromagnetic interference, *Bibliographies, Electromagnetic fields, Electromagnetic noise, Waveforms, Metrology.

The bibliography lists the publications of the personnel of the NBS Electromagnetic Fields Division in the period from January 1982 through December 1983. Topic headings include Antennas, Electromagnetic Interference, Noise, Waveform Metrology, and miscellaneous.

500,775
PB85-229961 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Semiconductor Devices and Circuits Div.
Improved Test Structure and Kelvin-Measurement Method for the Determination of Integrated Circuit Front Contact Resistance.
Final rept., J. A. Mazer, L. W. Linholm, and A. N. Saxena. 1985, 5p
Pub. in Jnl. of the Electrochemical Society 132, n2 p440-443 Feb 85.

Keywords: *Integrated circuits, Electrical resistance, Electric contacts, Measurement, Test equipment, Reprints.

The use of an improved microelectronic test structure and associated Kelvin measurement method for determining front contact resistance (circuit loading resistance) of a metal/semiconductor ohmic contact is described. The values of front contact resistance for aluminum/silicon contacts are determined using this Kelvin-cross contact resistance test structure and are compared with values determined by a two-terminal contact chain method and with values determined by a Kelvin voltage divider method. The values of front contact resistance using the Kelvin-cross structure and associated measurement method are shown to be less sensitive to photolithographic process variations and electrical measurement errors than those determined using the other two structures and measurement methods.

500,776
PB86-102381 Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Fields Div.
Screenroom Measurements of Antenna Factors.
Final rept., J. E. Cruz, and E. B. Larsen. Mar 85, 2p
Pub. in Proceedings of the IEEE (Institute of Electrical and Electronic Engineers) Instrumentation and Measurement Technology Conference, Tampa, Florida, March 20-22, 1985, p208.

Keywords: *Antennas, *Electromagnetic fields, Measurement, Anechoic chambers.

The measurement of electromagnetic fields in a shielded enclosure (screenroom) has serious problems because of uncertain antenna factors and multipath reflections from conductive surfaces. Most electromagnetic interference antennas at NBS are calibrated in a known field at an open field site using the standard antenna method. Because these antenna factors are not necessarily applicable for making measurements in a screenroom, the measurement errors are difficult to determine. This paper presents the results for antenna factors determined in a screenroom using the two-antenna method. These antenna factors are compared with antenna factors determined at an open field site and in an anechoic chamber. Experimental data are presented to show the variability of antenna factor as a function of frequency and location in the screenroom, thereby providing an indication of error bounds.

500,777
PB86-102688 PC A05/MF A01

National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Fields Div.
Near-Field Array of Yagi-Uda Antennas for Electromagnetic Susceptibility Testing.
Technical note, D. A. Hill, and G. H. Koepke. Jul 85, 84p NBS/TN-1082
Also available from Supt. of Docs as SN003-003-02669-7.

Keywords: *Antenna arrays, Yagi antennas, Electromagnetic fields, Electromagnetic susceptibility, Near field.

In electromagnetic susceptibility testing of electronic equipment, the ideal incident field is a plane wave. To approximate this condition, a seven-element array of Yagi-Uda antennas has been constructed and tested at a frequency of 500 MHz. The element weightings are determined by a near-field synthesis technique which optimizes the uniformity of the field throughout a rectangular test volume in the near field of the array. The amplitude and phase of the electric field have been measured throughout the test volume with a short dipole probe, and the agreement with the theory is excellent.

500,778
PB86-115680 PC A03/MF A01
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Fields Div.
Radio-Frequency Power Delivery System: Procedures for Error Analysis and Self-Calibration, M. Kanda, and R. D. Orr. Aug 85, 28p NBS/TN-1083
Also available from Supt. of Docs as SN003-003-02670-1.

Keywords: *Radio frequency power, Antennas, Error analysis, Calibrating.

An expression is developed for net power delivered to a load in terms of the indicated forward and reflected power and the system S-parameters and reflection coefficients. The dual directional coupler is treated as nonideal with power reflections assumed between all ports. The system itself is used to evaluate the major S-parameter terms in net power computation, and uncertainty in the computed power is derived from origins in the power meter readings and incompletely known S-parameters.

500,779
PB86-122801 Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div.
Automatic Frequency Response of Frequency-Modulated Generators Using the Bessel Null Method.
Final rept., J. R. Major, E. M. Livingston, and R. T. Adair. 1985, 23p
Sponsored by Army Communications-Electronics Command, Fort Monmouth, NJ.
Pub. in Proceedings of ARFTG Conference (24th), Columbia, MD., December 5-6, 1984, p131-153 Mar 85.

Keywords: *Signal generators, *Frequency response, Frequency modulation, Curve fitting, Frequency meters, Bessel null.

The paper describes a Bessel null technique to measure the frequency response of a frequency-modulated rf carrier and a program to automate frequency response measurements of signal generators with output frequencies from 0.450 to 2000 MHz. The measurements obtained using this technique are more accurate than those obtained by a highly trained technician using a manual system. Automated measurement of this process is desirable since the manual method is subject to the following problems: (1) excessive time; (2) error in finding the null; and (3) lack of assurance that the null is the first Bessel null. Automated measurements can be performed using a system controller, a spectrum analyzer, a function generator, and a voltmeter (all of which are compatible and controllable remotely).

500,780
PB86-122892 Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Fields Div.

Determination of Near-Field Correction Parameters for Circularly Polarized Probes.
Final rept., A. C. Newell, M. H. Francis, and D. P. Kremer. 1984, 29p
Pub. in Proceedings of Annual Conference of the Antenna Measurement Techniques Association, San Diego, CA., October 2-4, 1984, p3A3-1 - 3A3-29.

Keywords: *Antennas, *Antenna radiation patterns, Measurement, Far field, Circular polarization, Near field.

In order to accurately determine the far-field of an antenna from near-field measurements the receiving pattern of the probe must be known so that probe correction can be performed. When the antenna to be tested is circularly polarized, the measurements are more accurate and efficient if circularly polarized probes are used. Further efficiency is obtained if one probe is dual polarized to allow for simultaneous measurements of both components. A procedure used by the National Bureau of Standards for determining the plane-wave receiving parameters of a dual-mode, circularly polarized probe is described herein. First, the on-axis gain of the probe is determined using the three antenna extrapolation technique. Second, the on-axis axial ratios and port-to-port comparison ratios are determined for both the probe and source antenna using a rotating linear horn. Far-field pattern measurements of both amplitude and phase are then made for both the main and cross components.

500,781
PB86-124955 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Semiconductor Materials and Processes Div.
Hermetic Testing of Large Hybrid Packages.
Final rept., S. Ruthberg. 1982, 18p
Pub. in Proceedings of International Microelectronics Symposium, Reno, NV., November 15-17, 1982, International Jnl. of Hybrid Microelectronics 5, n2 p215-232.

Keywords: *Leak detectors, *Microelectronics, Semiconductor devices, Tests, *Hybrid circuits, *Hermetic seals, Krypton 85.

Hermetic testing is a routine operation in the microelectronics industry with millions of packages being screened each year. Yet disagreements in test results between supplier and user are common, different test methods provide different results for the same leak range on the same parts, results are dependent on package configuration, and the specified reject limits as set forth in the standards are somewhat arbitrary. The leak rate reject level for the larger package is considered from the viewpoint of moisture infusion rates, and their impact on test parameters is examined. Range, efficiency, and usefulness are examined for such popular test procedures as the helium leak detector, radioisotope, weight gain, and bubble methods as well as for others such as the tracer probe, differential pressure, and rapid cycle methods that are more appropriate for the larger package. The issues described above are discussed with the aid of graphical solutions and actual test data.

500,782
PB86-133436 Not available NTIS
National Bureau of Standards (NEL), Washington, DC. Semiconductor Devices and Circuits Div.
Sensitivity of SPICE Simulations to Input Parameter Variations.
Final rept., J. M. Cassard. 1983, 5p
Pub. in Proceedings of 1983 Custom Integrated Circuits Conference, Rochester, NY., May 23-25, 1983, p224-228.

Keywords: *Integrated circuits, *Simulators, Wafers, Simulation, Dynamic response, Sensitivity, CMOS, Chips(Electronics).

The paper presents examples of how well input parameters extracted from a test chip can predict the ac response of a dynamic circuit element on the same wafer. Simulation results show which model parameters are critical to performance. A comparison of measurement and simulation results is given and the importance of intra-chip and intra-wafer parameter variations is discussed.

Field 9—ELECTRONICS AND ELECTRICAL ENGINEERING

Group 9E—Subsystems

500,783

PB86-134889

(Order as PB86-134871, PC A09/MF A01)
National Bureau of Standards (NEL), Gaithersburg, MD. Electrosystems Div.

Digital Waveform Synthesis Techniques,

N. M. Oldham. Oct 85, 13p

Included in Proceedings of Seminar on Digital Methods in Waveform Metrology, p1-13 Oct 83.

Keywords: *Waveform generators, Digital systems, Synthesis.

Digital waveform generators provide an economical means for producing stable, high fidelity signals over a limited frequency range. Some theoretical properties and practical limitations have been described, with emphasis on sine wave reconstruction. Digital synthesis, however, is particularly suited to the construction of complex waveforms which are extremely difficult to produce by conventional analog means. Instrumentation is commercially available which allows the user to program arbitrary waveforms with 8-12 bit resolution at sampling frequencies up to 5 MHz.

500,784

PB86-138492

Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div.

Estimation of True Power Ratios in Six-Port Network Analyzers Using Diode Detectors.

Final rept.,

D. R. Holt, and C. A. Hoer. 1985, 2p

Pub. in Proceedings of IMTC '85 IEEE Instrumentation and Measurement Technology Conference, Tampa, Florida, March 20-22, 1985, p140-141.

Keywords: Network analyzers, Estimating, Detectors, Diodes.

A model for detector nonlinearity is included in the determination of six-port parameters without using additional standards. A computer simulation was performed assuming that the true power into each six-port detector is related to the power observed by the detector. Simultaneous estimation of the six-port and detector parameters is accomplished through a nonlinear least squares algorithm. Results of the simulation compare Gamma computed from corrected power readings and Gamma calculated from observed power readings.

500,785

PB86-139797

Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Fields Div.

Practical Optical Modulator and Link for Antennas.

Final rept.,

J. C. Wyss, and S. T. Sheeran. 1985, 6p

Pub. in Jnl. of Lightwave Technology LT-3, n2 p316-321 Apr 85.

Keywords: *Fiber optics transmission lines, Antennas, Electrooptics, Electromagnetic interference, Photodiodes, Reprints, Fiber optics.

The paper describes a practical application of a technique for coupling an antenna to a receiver using a passive fiber-optic link. This technique should avoid pickup and electromagnetic perturbations normally associated with the use of electrically conductive cables. Laser light (632.8 nm) is modulated at the antenna by an electrooptic lithiumtantalate crystal and is then transmitted with a fiber-optic cable to the receiver electronics. Using an avalanche photodiode, the amplitude modulated optical signal is converted to an electrical signal. The crystal is mounted directly on an antenna without amplifiers or other electrically powered components.

500,786

PB86-139854

Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Semiconductor Materials and Processes Div.

Total Dose Effects on Circuit Speed Measurements.

Final rept.,

M. D. Lantz, and K. F. Galloway. 1983, 6p

Pub. in IEEE Trans. Nuclear Science 30, n6 p4264-4269 1983.

Keywords: *Integrated circuits, *Radiation effects, Ionizing radiation, Radiation dosage, Time lag, Metal oxide transistors, Reprints, *Physical radiation effects, Delay, CMOS.

Measurements of propagation delay as a function of total ionizing dose were made using ring-oscillators, inverter chains, and NAND chains fabricated on the same CMOS test chip. The data illustrate the impact of the bias conditions of the MOS transistors during irradiation on the propagation delay time of the circuits. The data show no difference in propagation delay time for the three circuit types if comparable bias conditions are maintained during radiation exposure. The threshold voltage shift of the n-channel transistor in the 'ON' state appears to be the dominant factor controlling the decrease in propagation delay as the total dose increased. The ultimate failure of the test circuits is due to the shift of the n-channel transistors to a negative threshold voltage.

500,787

PB86-156585

PC A08/MF A01
National Bureau of Standards, Gaithersburg, MD.

Electrical Performance Tests for Audio Distortion Analyzers.

Final rept.,

O. B. Laug, G. N. Stenbakken, and T. F. Leedy. Nov 85, 158p NBSIR-85/3269

Sponsored by Army Communications-Electronics Command, Fort Monmouth, NJ.

Keywords: *Distortion, *Sound analyzers, High pass filters, Low pass filters, Performance tests.

Electrical performance test procedures for audio distortion analyzers were developed by the National Bureau of Standards for the U.S. Army Communications-Electronics Command. The report provides detailed, step-by-step test procedures that are based on specifications supplied by the Army for purposes of evaluating audio distortion analyzer bid samples. The report discusses the philosophy of each measurement procedure with a view toward providing an understanding of the basic metrology required to perform the measurements. In addition, the sources of measurement error are discussed. The primary applications and basic principles of modern audio distortion analyzers are also presented.

500,788

PB86-164357

PC A05/MF A01
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Fields Div.

Development of Near-Field Test Procedures for Communication Satellite Antennas. Phase 1, Part 1,

A. C. Newell, and A. G. Repjar. Sep 85, 82p NBSIR-85/3031

Keywords: *Spacecraft antennas, Electromagnetic fields, Antennas, Tests, Measurement, Communication satellites, Near field.

The purpose of the program is to define and further develop the capabilities of near-field antenna test techniques, specifically for the requirements associated with the development and verification testing of reconfigurable, multibeam, frequency reuse, commercial satellite antennas. Phase I, Part 1 gives a general survey, definition, and description of near-field and compact range measurement methods as they apply to satellite antenna systems testing. Each of these methods is evaluated to determine how well they meet the measurement requirements. Included for each technique is a summary of the measurement method, discussions on probe correction and data processing, measurement hardware considerations, a results available section, and measurement accuracy and range certification considerations. The basis for the choice of the best measurement technique is established with the planar near-field measurement method receiving the best score for the directive antennas considered.

500,789

PB86-169083

PC A04/MF A01
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Fields Div.

Site Attenuation,

R. G. FitzGerrell. Nov 85, 51p NBS/TN-1089

Also available from Supt. of Docs as SN003-003-02708-1.

Keywords: *Antennas, Attenuation, Measurement, Dipole antennas.

Site attenuation is a measure of performance of an open test site used at frequencies below about 1 GHz for antenna calibration and equipment emission and susceptibility testing. These sites typically consist of a

large, obstruction-free ground plane and the hemisphere above it. Site attenuation of an ideal site is calculated and compared to data measured using the 30 m by 60 m NBS ground screen.

10. ENERGY CONVERSION (NON-PROPULSIVE)

10A. Conversion Techniques

500,790

DE85000385

PC A07/MF A01
National Bureau Standards (NEL), Boulder, CO. Chemical Engineering Science Div.

Thermophysical Properties of Working Fluids for Binary Geothermal Cycles. Final Report.

D. E. Diller, J. S. Gallagher, B. Kamger-Parsi, G. Morrison, and J. M. H. Levelt Sengers. Jul 84, 150p NBSIR-85/3124-DOE, DOE/RA-50241-11

Contract AT01-80RA50241

Portions are illegible in microfiche product. Original copy available until stock is exhausted.

Keywords: *2-Methylbutane, *2-Methylpropane, Binary-Fluid Systems, Geothermal power plants, Hydrocarbons, Mixtures, Scaling laws, Thermodynamic properties, Viscosity, Working fluids, ERDA/150802, ERDA/360603.

The following are presented: thermodynamic properties of isobutane and isobutane-isopentane mixtures; a scaled fundamental equation for mixtures of isobutane and isopentane near gas-liquid critical line; and viscosities of hydrocarbons and their mixtures. (ERA citation 10:006697)

500,791

PB85-170678

Not available NTIS
National Bureau of Standards, Gaithersburg, MD.

Economics of Energy Management.

Final rept.,

R. T. Ruegg. Sep 84, 11p

Sponsored by Department of Energy, Washington, DC. Pub. in Heat/Piping/Air Conditioning 56, n9 p63-73 Sep 84.

Keywords: *Economic analysis, Cost analysis, Economic factors, Return on investment, Decision making, Reprints, *Energy management, Life cycle costs.

This article promotes effective energy management by guiding the reader to ask the right economic questions, evaluate the cost effectiveness of alternative investments and find assistance along the way. It provides a tabular overview of various methods of economic evaluation, provides an anatomy of life-cycle costing, advises on compiling data and making assumptions, and guides the reader through successive levels of the decision-making process.

500,792

PB85-183374

PC A03/MF A01
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.

Self-Heating to Ignition Measurements and Computation of Critical Size for Solar Energy Collector Materials.

Final rept.,

J. J. Loftus. Mar 85, 39p NBSIR-85/3122

Sponsored by Department of Energy, Washington, DC.

Keywords: *Plywood, *Cellular plastics, *Ignition, Critical temperature, Hazards, Polyurethane resins, *Solar collectors.

Kinetic constants of the self-heating reaction were determined for plywood, a retardant treated plywood, and eight samples of polyurethane foam representing pos-

sibly two different kinds of foam materials. Under the assumption that self-heating follows a first order reaction, these constants were used to calculate the critical half thickness of slabs of these materials for surface temperatures likely to be experienced during long term use in solar energy collectors. Based on these calculations, estimates are provided on the self-heating or ignition hazards associated with the size and use of these materials in solar energy systems.

500,793
PB85-187607 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Using Infrared Thermography for Industrial Energy Conservation.

Final rept.,
T. P. Sheahan, Y. Y. Haimes, and M. A. H. Ruffner.
1979, 42p
Pub. in Proceedings of Energy Auditing Conservation: Methods, Measurements, Management, and Case Studies Conference, Cleveland, OH., March 14, 1979, p59-100.

Keywords: *Infrared thermal detectors, *Industrial heating, *Thermography, Furnaces, Heat loss, Temperature distribution, Measurement, Heat balance, Ovens, Numerical analysis, Measuring instruments, *Energy conservation.

The experimental techniques of infrared thermography have been used in factories to locate heat losses from furnaces, ovens and similar industrial equipment. Infrared thermography data have been used to generate temperature maps of furnaces, based on precise measurements made with a calibrated instrument. From these temperature maps, we have calculated total radiation losses, and have estimated convective heat losses as well. By combining these calculations with other numerically estimated losses, we have carried out a full heat-balance on a furnace, leaving no 'unaccounted' amount as in typical calculations of the past. This paper explains how infrared thermography works, and gives a variety of examples from both qualitative applications (leakage, hotspot identification, etc.) and quantitative measurements of heat balances.

500,794
PB85-196582

(Order as PB85-196541, PC A07/MF A01)
Florida Univ., Gainesville.
Microcomputer Design Tool to Aid Construction Professionals to Comply with the Florida Model Energy Efficiency Code,
G. D. Cook. Apr 85, 26p
Sponsored by National Bureau of Standards (NEL), Gaithersburg, MD. Center for Building Technology, and National Conference of States on Building Codes and Standards, Inc., Herndon, VA.
Included in Research and Innovation in the Building Regulatory Process: Proceedings of the NBS/NCSBCS Joint Conference (6th), Technical Seminar on Streamlined Administrative Procedures, Computers in Construction, and Fire Safety Technology held at Denver, Colorado on September 11, 1984, p45-70 Apr 85.

Keywords: Residential buildings, Computer programs, Florida, *Energy efficiency standards, Compliance, Computer aided design, Energy consumption.

This paper discusses the development and use of an Apple II+ compatible computer program that calculates the residential Energy Performance Index (EPI) under Section 9 of the Florida Model Energy Efficiency Code. The program was developed as a design tool for builders, engineers, architects, and others in the construction field desiring to achieve cost effective and superior residential energy performance under the code.

500,795
PB85-197465 Not available NTIS

National Bureau of Standards, Gaithersburg, MD.
Method to Abbreviate Hourly Climate Data for Computer Simulation of Annual Energy Use in Buildings.
Final rept.,
E. Arens, L. Flynn, and D. Nall. 1979, 5p
Pub. in Proceedings of National Passive Solar Conference (4th), Kansas City, MO., October 3-5, 1979, p282-286.

Keywords: *Buildings, Statistical analysis, Data, Climate, Thermal analysis, Predictions, Computerized simulation, *Energy consumption.

A building's future energy performance is commonly estimated by simulating its thermal behavior over a

'typical' year representative of the most statistically probable future climate. A technique is presented to abbreviate the hourly climate data used in such analysis. It is incorporated in a computer program that selects from each month of a full year's climate record a shorter segment that represents the month. The technique's empirical basis is reported, followed by the results of various tests of its effectiveness at representing full-length data. The results suggest how far one can actually abbreviate climate data before the thermal lag of the building begins to distort predicted energy. The paper finally discusses the potential for using the technique for other applications, such as creating typical years and synthesizing hourly data for sites for which there is only summarized data.

500,796
PB85-202133 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
General Illuminance Model for Daylight Availability.

Final rept.,
G. Gillette, W. Pierpoint, and S. Treado. 1984, 11p
Pub. in Jnl. of the Illuminating Engineering Society 13, n4 p330-340 Jul 84.

Keywords: *Daylight, *Illuminance, Solar radiation, Availability, Intensity, Reprints, Sky radiation.

Based largely on extensive sky measurements at the National Bureau of Standards, plots have been made of sky and sun illuminances as functions of solar altitude and time of year. Comparisons have also been made of how these plots relate to values currently used by the I.E.S., and against similar measurements made by others within the U.S. and abroad. A value of extraterrestrial illuminance and its atmospheric attenuation have also been developed using related solar principles. Algebraic expressions have been prepared for obtaining, (1) the extraterrestrial illuminance, (2) direct normal solar illuminance inside the atmosphere, and (3) horizontal sky illuminance without the sun. While the extraterrestrial and direct normal solar values have been found to be functions also of Julian date, all plots seem to show a consistent correlation with solar altitude.

500,797
PB85-207942 Not available NTIS

National Bureau of Standards (NEL), Gaithersburg, MD. Building Equipment Div.
Criteria for Mechanical Energy Saving Retrofit Options for Single-Family Residences.
Final rept.,
E. Kwellner, and S. Silberstein. Aug 84, 15p
Sponsored by Department of Energy, Washington, DC. Pub. in Proceedings of ACEEE 1984 Summer Study on Energy Efficiency in Buildings, New and Existing Single-Family Residences, Santa Cruz, CA., August 15-23, 1984, Volume B, pB-144-B-158.

Keywords: *Residential buildings, Heat recovery, Cost analysis, Space heating, Hot water heating, Air conditioning, *Retrofitting, *Energy conservation.

The report estimates energy savings, and provides performance and selection criteria, standards, and installed costs for mechanical equipment options for single-family homes; all from prior studies reported in the literature. Performance and selection criteria are presented as advantages, disadvantages and limitations for each option. Four broad categories of energy-saving mechanical options were investigated: space heating, water heating retrofit options, heat pump water heaters, and recovery of central air conditioner waste heat by desuperheaters. Gas- and oil-fueled forced-air furnaces and hydronic (hot water) space-heating equipment were treated in the report.

500,798
PB85-227635 Not available NTIS

National Bureau of Standards (NEL), Gaithersburg, MD. Operations Research Div.
Life-Cycle Costing with the Microcomputer.
Final rept.,
S. R. Petersen, and H. E. Marshall. Jun 85, 6p
Pub. in ASTM (American Society for Testing and Materials) Standardization News 13, n6 p36-41 Jun 85.

Keywords: *Buildings, Benefit cost analysis, Economic analysis, Investments, Rates(Costs), Return on investment, Revisions, Reprints, *Life cycle costs, *Energy conservation, Computer applications, Retrofitting, Microcomputers, User manuals(Computer programs), Modifications.

The Building Life-Cycle Cost (BLCC) microcomputer program and its user's guide are an adjunct to the standard economic methods developed by ASTM for evaluating buildings. The article describes how the program/user's guide can be used to facilitate application of the program to a real building investment problem involving envelope and equipment modifications for energy conservation.

500,799
PB85-230837 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Measured Data on Energy Consumption in Single Family Detached Homes Across the United States.
Final rept.,
R. Crenshaw. 1980, 6p
Sponsored by Department of Energy, Washington, DC. Pub. in Proceedings of the National Passive Solar Conference (5th), Amherst, Massachusetts, October 19-26, 1980, p670-674.

Keywords: *Residential buildings, Urban areas, Solar energy, Heat balance, Statistical data, *Energy consumption, Energy conservation, Weatherization, Retrofitting.

Two hundred and twenty houses were selected in 14 cities across the country to be weatherized and evaluated. Infiltration rates, mechanical efficiencies, building dimensions, solar data and energy consumption data before and after weatherization were collected on each of these houses. This paper presents the before weatherization data on 33 houses at Charleston, S.C., Colorado Springs, CO, and Fargo, N.D. It also compares modified steady-state heat balance calculations which include solar data to the utility data of each of these houses.

500,800
PB86-112729 Not available NTIS

National Bureau of Standards, Gaithersburg, MD.
Industrial/Commercial Insulation for Mechanical Systems Applications.
Final rept.,
F. J. Powell. 1981, 3p
Pub. in Proceedings of Energy Technology Conference and Exposition (8th), Washington, DC., March 9-11, 1981, p547-549.

Keywords: *Thermal insulation, *Energy conservation.

The article gives the potential for energy savings and the justifications for using industrial/commercial thermal insulations on mechanical systems and equipment such as pipes, ducts, tanks, vessels, boilers, furnaces, and surfaces at which heat is transferred within the temperature range of -300F to +2800F. A potential savings of 250 million equivalent barrels of oil per year exists with 104 million equivalent barrels per year by improving the insulation on industrial steam process pipes alone. For pipes, this would cost \$6.2 billion with a payback in 30 months. Activities that feature the reduction of heat gain or loss in existing or new mechanical systems and their components by application of cost effective levels of thermal insulation and from effective installation, operation, and maintenance practices are suggested.

500,801
PB86-113610 Not available NTIS

National Bureau of Standards (NEL), Gaithersburg, MD. Structures Div.
Development of Standards for Evaluating Solar Absorber Materials.
Final rept.,
L. Masters, and D. Waksman. 1979, 21p
Sponsored by Department of Energy, Washington, DC. Office of Conservation and Solar Energy.
Pub. in Proceedings of the American Electroplaters Society Coatings for Solar Collectors Symposium (2nd), St. Louis, MO., October 16-17, 1979, 21p.

Keywords: *Standards, *Solar absorbers, Solar space heating, Solar cooling systems, Solar collectors.

Absorber materials used in solar heating and cooling systems absorb energy from the sun and convert it to thermal energy. It is essential that materials used for this purpose be durable for extended periods of time. However, the environment in which absorber materials are used can cause rapid degradation. Numerous problems in solar energy systems have clearly shown the need for standards by which solar absorber materials and other materials can be evaluated. The Center for Building Technology of the National Bureau of

Field 10—ENERGY CONVERSION (NON-PROPULSIVE)

Group 10A—Conversion Techniques

Standards is performing research, under Department of Energy sponsorship, to develop the measurement technology needed for standards, both at the solar collector level and the functional materials level. This paper addresses the ongoing research, the findings to date, and draft standards that have resulted from the research.

500,802
PB86-119211 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Structures Div.
Laboratory Simulated Service Testing of Flat Plate Solar Heat Transfer Liquid Containment Systems.
Final rept.,
P. W. Brown. 1980, 8p
Sponsored by Department of Energy, Washington, DC. Office of Solar Applications and Commercialization. Pub. in Proceedings of International Corrosion Forum Devoted Exclusively to the Protection and Performance of Materials, Chicago, IL., May 3-7, 1980, p102.1-102.8.

Keywords: Accelerated tests, Simulators, Ethylene, Glycols, *Solar collectors, *Heat transfer fluids, Flat plate collectors.

The design of an accelerated test simulative of the operation of a solar collector system requires consideration of a variety of possible design and operating parameters. These include operating and stagnation temperatures, flow rate, mode of heat transfer and degree of aeration. Cognizant of these parameters, a simulated service test, which allows stagnant empty and full conditions to be simulated at temperatures either above or below the boiling temperature of the heat transfer liquid, has been developed. The chemical and thermal stabilities of ethylene and propylene glycol have also been examined.

500,803
PB86-123049 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Testing Solar Collector Materials Durability by Integrated Day-Long Stagnation Temperature Measurements.
Final rept.,
W. C. Thomas, A. G. Dawson, and D. Waksman. 1983, 7p
Pub. in Proceedings of ASME (American Society of Mechanical Engineers) Solar Energy Division Annual Conference (5th), Orlando, FL., April 18-21, 1983, p301-307.

Keywords: *Solar collectors, Materials tests, Durability, Tests, Temperature measurement, Degradation.

Measurements of the maximum temperatures reached by solar energy absorbing surfaces provide a useful method for detecting possible degradation in the optical and heat transfer properties of materials used in collectors. The test method is based on measuring the absorber temperature continuously over a period of several days along with total daily solar irradiation. The absorber temperature rise above ambient is integrated to determine daily values. The investigation shows that the all-day integration method is a viable approach which has advantages over alternative test methods based on steady-state measurements of either absorber stagnation temperature or collector energy output.

500,804
PB86-124864 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Building Physics Div.
Field Evaluation of Aerial Infrared Surveys for Residential Applications.
Final rept.,
S. J. Treado, and D. M. Burch. 1982, 7p
Pub. in Proceedings of the Society of Photo-Optical Instrumentation Engineers, Ottawa, Ontario, September 1-4, 1981, Paper in Thermal Infrared Sensing Applied to Energy Conservation in Building Envelopes (Thermosense IV) 313, p28-34 1982.

Keywords: *Residential buildings, Aerial surveys, Roofs, Thermal analysis, Remote sensing, *Infrared thermography, Energy conservation.

The effectiveness of aerial infrared thermography as an energy audit procedure for residences having pitched ventilated roofs is investigated. Three adjacent unoccupied houses were instrumented to provide ground-truth comparison data under various weather conditions. Factors affecting the accuracy of this technique

are identified and analyzed, and guidelines are presented concerning the recommended use of aerial infrared thermography as a procedure for assessing the thermal performance of residences.

500,805
PB86-133493 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Building Physics Div.
Role of Thermography in the Assessment of the Thermal Integrity of Federal Office Buildings.
Final rept.,
Y.-M. Chang, and R. A. Grot. 1984, 9p
Pub. in Proceedings of SPIE (Society of Photo-Optical Instrumentation Engineers) International Conference on Thermal Infrared Sensing for Diagnostics and Control (Thermosense 6), Oak Brook, IL., October 2-5, 1983, v446 p47-55 1984.

Keywords: *Office buildings, Ground based detectors, Thermal analysis, *Infrared thermography, Energy conservation, Federal buildings.

Results were presented from ground-based infrared thermographic studies performed by NBS on eight Federal Office Buildings. Infrared thermography was used to observe the thermal anomalies in those buildings, as part of a diagnostic program to evaluate the thermal integrity of building envelopes. Thermographic data were collected via complete exterior scannings and selected interior scannings at regions where thermal defects were identified or suspected during the outside inspections. Analysis from thermographic inspections with examples of defects found in some of these buildings are also included. The potential applications of the diagnostic procedures to both new and existing buildings are discussed.

500,806
PB86-139987 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Structures Div.
Wind Loads on Solar Collectors: Development of Design Guidelines.
Final rept.,
T. A. Reinhold. 1981, 8p
Pub. in Proceedings of U.S. National Conference on Wind Engineering Research (4th), Seattle, Washington, July 26-29, 1981, p313-320.

Keywords: Wind pressure, Design, Guidelines, Structural engineering, *Solar collectors.

Measurements obtained from model and full-scale tests are used to develop guidelines for determining minimum design wind loads on solar collectors. The approach followed is to use the proposed 1980 draft revisions to ANSI A58.1, 'Building Code Requirements for Minimum Design Loads in Buildings and Other Structures' as a base document. Guidelines are then developed which will extend the use of tables in the 1980 Draft ANSI A58.1 Provisions to the specification of minimum wind loads on solar collectors in a variety of installations. This paper includes comparisons of model with full-scale test results. Also included are comparisons of roof and wall pressures specified in the 1980 Draft ANSI A58.1 Provisions with corresponding measured pressures. These comparisons are used to evaluate the validity of the model test results and to develop pressure coefficients compatible with the 1980 Draft ANSI A58.1 Provisions.

500,807
PB86-153848 PC A02/MF A01
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Building Technology.
Opportunities for Full-Scale Testing of Residential Building Interactions in Environmental Chambers.
A. K. Persily. Dec 85, 21p NBSIR-85/3194
Sponsored by Department of Energy, Washington, DC. Architectural and Engineering Systems Branch.

Keywords: *Residential buildings, Test chambers, Testing, Performance evaluation, Energy conservation.

The report focuses on opportunities for full-scale testing of residential building interactions in environmental chambers, where one has control of weather conditions and occupant effects. Such research will increase our understanding of the physical nature of these interactions and their effects on energy use, comfort, cost, and other factors. In the report the authors review past and current research in the area of full-scale testing in environmental chambers and other related work. Based on the review, further research is

proposed in several important areas of residential building performance.

10B. Power Sources

500,808
PB85-184893 PC A03/MF A01
National Bureau of Standards (NEL), Gaithersburg, MD. Electrosystems Div.
Development of Power System Measurements - Quarterly Report July 1, 1984 to September 30, 1984.
R. E. Hebner. Mar 85, 40p NBSIR-85/3111
See also DE84-017001.

Keywords: *Power transmission lines, *Sulfur hexafluoride, Measurement, Electric fields, Magnetic fields, Electrical insulation, Interfaces, Insulating oil, Electric discharges, *HVDC systems.

The report documents the progress on four technical investigations sponsored by the Department of Energy and performed by or under a grant from the Electrosystems Division, the National Bureau of Standards. The work described covers the period from July 1, 1984 to September 30, 1984. The report emphasizes the errors associated with measurements of electric and magnetic fields, the properties of corona in compressed SF6 gas, the measurement of interfacial phenomena in transformer oil, and the measurement of dielectric properties on nanosecond time scales.

500,809
PB85-195964 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Summit Plaza Total Energy Demonstration: Four Years of Operating Experience.
Final rept.,
J. D. Ryan. 1979, 17p
Sponsored by Department of Housing and Urban Development, Washington, DC. Office of Policy Development and Research.
Pub. in International Total Energy Congress (2nd), Copenhagen, Denmark, October 8, 1979, Part 1, p39-55.

Keywords: Residential buildings, Heat recovery, District heating, Diesel engines, *Total energy systems, Cogeneration.

The paper presents a summary of the measured data and results of the U.S. Department of Housing and Urban Development's (HUD) Total Energy demonstration project at the Summit Plaza complex in Jersey City, N.J. Operation of the plant began in January, 1974. The National Bureau of Standards (NBS) monitored and collected data on the plant through October, 1978. This paper presents summary data on the operating thermal performance of plant components including diesel engine-generators, heat recovery, boilers, chillers, district heating system, etc. Also presented are electrical service reliability data including a comparative analysis with utility data. Environmental data (stack emissions and measured ground-level air quantity) and economic data (capital cost and operating and maintenance costs) are also included.

10C. Energy Storage

500,810
PB85-201945 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Neutron Powder Diffraction Study of alpha- and beta-PbO2 in the Positive Electrode Material of Lead-Acid Batteries.
Final rept.,
A. Santoro, P. D'Antonio, and S. M. Caulder. 1983, 9p
Pub. in Jnl. of the Electrochemical Society 130, n7 p1451-1459 Jul 83.

Keywords: *Lead acid batteries, *Neutron diffraction, *Electrochemistry, *Electrodes, *Cations, Molecular structure, Lead oxides, Reprints.

A neutron powder diffraction study of alpha- and beta-PbO2, both chemically prepared and electrochemically

formed in cycled battery plates, was carried out to correlate the electrochemical activity of the lead-acid battery with the atomic arrangement of the electrode constituents. The authors results indicate that there are neither lead nor oxygen deficiencies, and therefore, any hydrogen which is present must be accompanied by a reduction of $Pb(+4)$. In addition, they have observed a significant increase in the lattice parameter a of β - PbO_2 in cycled battery electrodes relative to the value in chemically prepared β - PbO_2 . No change in the c parameter, however, was detected. This suggests that the OH groups present in the structure are probably oriented perpendicular to c along (110). This configuration is similar to that observed in SnO_2 .

500,811
PB86-105699 PC A03/MF A01
Scientific Consulting Services, Pullman, WA.
Mathematical Model for the Distribution of the Long-Term Efficiency of Phase-Change Materials and Its Application in Heat-Storage.
S. C. Lowell, and S. C. Saunders. 25 Aug 85, 41p
NBS/GCR-85-492
Sponsored by National Bureau of Standards (NEL), Gaithersburg, MD. Center for Building Technology, and Department of Energy, Washington, DC. Office of Solar Heat Technologies.

Keywords: *Mathematical models, *Heat storage, *Phase transformation, Performance evaluation, Glauber's salt, *Phase change materials.

A mathematical model for the degradation in the thermal performance of a salt hydrate phase change storage system is discussed.

11. MATERIALS

11A. Adhesives and Seals

500,812
PB85-203578 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.
Safety Considerations, Oral and Systemic.
Final rept.,
R. L. Bowen, N. W. Rupp, and W. G. de Rijk. 1984, 3p
Sponsored by American Dental Association Health Foundation, Chicago, IL.
Pub. in Jnl. of Dental Education 48, n2 p32-34 1984.

Keywords: *Dental materials, *Sealants, *Polymeric films, Performance evaluation, Preventive medicine, Decay, Reprints.

A survey of the literature shows no test results in vitro or in vivo that contraindicates the use of pit and fissure sealant resins. The consensus of the authors given here is based not only on a thorough literature search but also on many years of first-hand experience with these materials. Furthermore, during the last decade during which many hundreds of thousands of applications of sealants have been made by other dentists together with their appropriately-trained auxiliary personnel, there have been no reports of untoward reactions either in the patients receiving the treatments or those administering them. There should be more widespread use of this valuable prevention method, which together with the proper use of fluorides, could nearly eliminate dental decay.

500,813
PB86-112182 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.
Viscoelastic Fracture Behaviour for Different Rubber-Modified Epoxy Adhesive Formulations.
Final rept.,
D. L. Hunston, and G. W. Bullman. Apr 85, 6p
Pub. in International Jnl. of Adhesion and Adhesives 5, n2 p69-74 Apr 85.

Keywords: *Viscoelasticity, *Epoxy resins, *Adhesives, *Fracture tests, Elastomers, Rheology properties, Reprints.

The viscoelastic fracture behaviour of various rubber-modified epoxy formulations was analysed using a time-temperature superposition approach. The shift factors for all of these systems were quite similar. In addition, an equivalent analysis of yield stress data was performed for one of the samples; it gave shift factors similar to those from the fracture experiments thus indicating a close correlation between yield and toughening. A simple empirical equation was found to describe the fracture data for all the materials and, consequently, the parameters in this equation provide a good method to characterize the fracture behaviour and to compare different materials.

11B. Ceramics, Refractories, and Glasses

500,814
PB85-179067
(Order as PB85-179042, PC A06/MF A01)
National Bureau of Standards, Gaithersburg, MD. Center for Materials Science.
Controlled Indentation Flaws for the Construction of Toughness and Fatigue Master Maps.
R. F. Cook, and B. R. Lawn. 30 Aug 84, 13p
Sponsored by Office of Naval Research, Arlington, VA. Prepared in cooperation with New South Wales Univ., Kensington (Australia).
Included in Jnl. of Research of the National Bureau of Standards, v89 n6 p453-465 Nov-Dec 84.

Keywords: *Nondestructive testing, *Ceramics, *Toughness, *Fatigue(Materials), Glasses.

A simple and economical procedure for accurate determinations of toughness and lifetime parameters of ceramics is described. Indentation flaws are introduced into strength test pieces, which are then taken to failure under specified stressing and environmental conditions. By controlling the size of the critical flaw, via the contact load, material characteristics can be represented universally on 'master maps' without the need for statistical considerations. This paper surveys both the theoretical background and the experimental methodology associated with the scheme. The theory is developed for 'point' flaws for dynamic and static fatigue, incorporating load explicitly into the analysis. A vital element of the fracture mechanics is the role played by residual contact stresses in driving the cracks to failure. Experimental data on a range of Vickers-indented glasses and ceramics are included to illustrate the power of the method as a means of graphic materials evaluation. It is demonstrated that basic fracture mechanics parameters can be measured directly from the slopes, intercepts and plateaus on the master maps, and that these parameters are consistent, within experimental error, with macroscopic crack growth laws.

500,815
PB85-183234 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Inorganic Materials Div.
Measurement of Thin-Layer Surface Stresses by Indentation Fracture.
Final rept.,
B. R. Lawn, and E. R. Fuller. 1984, 7p
Pub. in Jnl. of Materials Science 19, p4061-4067 1984.

Keywords: *Glass, *Brittleness, *Stresses, Measurement, Surface properties, Indentation, Fractures(Materials), Reprints.

A model is developed for evaluating stresses in the surfaces of brittle materials from changes in indentation crack dimensions. The underlying basis of the model is a stress intensity formulation incorporating the solution for a penny-like crack system subjected to a constant stress over a relatively thin surface layer. Results from a previous study of surface damage in proton-irradiated glass are used to illustrate the scope of the method. The indentation fracture analysis also provides some fresh insight into the susceptibility of brittle surfaces to spontaneous cracking. Implications of the study concerning the potential effect of surface stresses on mechanical properties, such as strength, erosion and wear, are briefly discussed.

500,816
PB85-183291 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Inorganic Analytical Research Div.
Microscale Homogeneity and Compositional Profiling of Borosilicate Glass Materials.
Final rept.,
J. W. Mitchell, J. E. Riley, and B. S. Carpenter. 1983, 9p
Pub. in Mikrochimica Acta III, p253-261 1983.

Keywords: *Borosilicate glass, *Glass, *Boron, Non-destructive tests, Optical fibers, Measurement, Reprints.

The instrumental analytical methods most widely used for providing information on the microscale homogeneity and depth profile distribution of major elements have deficiencies for characterizing borosilicate glasses. Several nuclear methods provide particularly specific, high sensitivity, and high resolution detection of boron. Thermal neutron bombardment with detection of promptly emitted alphas using silicon surface barrier detectors provides depth profile information on trace boron levels. The alternative, determination of boron by detecting emitted alpha particles by the track counting technique, is particularly attractive for establishing compositional homogeneity of trace boron distribution. This paper describes the use of the method for the detection of boron when present as a major constituent. The examples selected to demonstrate applicability of the method include characterization of commercial glasses, synthesized rods, and optical fibers. The potential of the nuclear track counting technique as a new method for quantitative non-destructive determination of boron as a major constituent is also being assessed in continuing work.

500,817
PB85-183309 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Inorganic Materials Div.
Deformation-Induced Crack Initiation by Indentation of Silicate Materials.
Final rept.,
H. Multhopp, B. R. Lawn, and T. P. Dabbs. 1984, 13p
Sponsored by Office of Naval Research, Arlington, VA. Pub. in Deformation of Ceramic Materials II, p681-693 1984.

Keywords: *Glass, *Silicon dioxide, *Quartz, *Crack initiation, Indentation, Kinetics, Reprints.

The micromechanics of radial crack initiation produced in indentation of soda-lime glass, fused silica and quartz are discussed in terms of a two-step, nucleation and growth model. Particular attention is focussed on the strong rate effects in the presence of environmental water, as manifested by a tendency to delayed crack pop in with decreasing contact duration. Microscopic examination of the indentations indicates that deformation 'shear faults', which accommodate the intense strains associated with the penetrating indenter, control the kinetics of the initiation process. The geometrical constraints which determine the stress concentrations for crack nucleation from these faults are structure-sensitive.

500,818
PB85-183408 PC A03/MF A01
National Bureau of Standards, Gaithersburg, MD. Inorganic Materials Div.
Estimation of Power-Law Creep Parameters from Bend Test Data.
T. J. Chuang. Feb 85, 44p NBSIR-85/2997
Contract DE-AI05-80OR20679
Sponsored by Air Force Office of Scientific Research, Bolling AFB, DC.

Keywords: *Ceramics, *Creep properties, Creep tests, Aluminum oxide, Applications of mathematics.

Power-law creep parameters of brittle ceramic materials are commonly deduced from load-point displacement data generated by four-point bend experiment, under the assumption that tensile and compressive behaviors obey the same constitutive law. However, thanks to different roles played by microcracking and cavitation, it is now well recognized that this premise on occasions may not be valid. The present paper undertakes an analysis which takes the differences into account. Governing equations are first derived for the locations of neutral axis of a beam under bending and for the creep responses in terms of both curvature rate

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and load point displacement rate as functions of the applied moment and power-law creep parameters. Numerical solutions are obtained for any given set of materials constants over a wide range of applied moments.

500,819

PB85-184794

Not available NTIS
National Bureau of Standards, Gaithersburg, MD.

Powder Processing of Potassium Aluminosilicates.

Final rept.,

L. P. Cook. 1982, 9p

Sponsored by Metallurgical Society of AIME, Warrendale, PA., and American Ceramic Society, Columbus, OH. Basic Science Div.

Pub. in Proceedings of Symposium on Metal and Ceramic Powers, Louisville, KY., October 12-14, 1981, Processing of Metal and Ceramic Powders, p137-145, 1982.

Keywords: *Densification, Ceramics, Sintering, Processing, *Potassium aluminosilicates.

Two processing alternatives have been investigated for overcoming the poor densification obtained during sintering of potassium aluminosilicates: 1--reaction sintering, employing KAlSi_2O_6 glass and KAlO_2 in the proper proportions to yield KAlSi_2O_6 or KAlSiO_4 and 2--use of submicron-sized single phase powders of KAlSi_2O_6 and KAlSiO_4 . Method 2 yields densities approaching 90 percent theoretical density for both KAlSi_2O_6 and KAlSiO_4 , provided powder particle sizes are below a certain threshold. Data describing the kinetics of these enhanced densifications at 1400°C have been obtained.

500,820

PB85-184810

Not available NTIS
National Bureau of Standards, Gaithersburg, MD.

Microcrack Healing During the Temperature Cycling of Single Phase Ceramics.

Final rept.,

E. D. Case, J. R. Smyth, and O. Hunter. 1983, 24p

Grant NSF-DMR78-01584

Pub. in Proceedings of the International Symposium on the Fracture Mechanics of Ceramics, University Park, PA., July 15-17, 1981, Surface Flaws, Statistics, and Microcracking, v5 p507-530 1983.

Keywords: *Ceramics, *Heat treatment, Magnesium titanates, Aluminum oxide, Cooling curves, Acoustic resonance, Measurement, Temperature, Modulus of elasticity, Meetings, Extrapolation, *Microcracks, Gadolinium oxides.

The healing of microcracks in single phase Al_2O_3 , Gd_2O_3 , and MgTi_2O_5 was studied by measuring Young's modulus versus temperature via a sonic resonance technique. Similar data was examined for Eu_2O_3 , Nb_2O_5 and HfO_2 . For a variety of grain sizes for each material, the linear portions of the modulus-temperature cooling curves were extrapolated to room temperature. These extrapolated modulus values $Y_{\text{sub RT}}$, were corrected to zero porosity ($Y_{\text{sub C}}$) by empirical modulus-porosity relations.

500,821

PB85-187425

Not available NTIS
National Bureau of Standards, Gaithersburg, MD.

Effect of Corrosion Processes on Subcritical Crack Growth in Glass.

Final rept.,

C. J. Simmons, and S. W. Freiman. 1981, 4p

Pub. in Jnl. of American Ceramics Society 64, n11 p683-686 1981.

Keywords: *Glass, *Crack propagation, Corrosion, Fracture properties, Reprints, Fracture(Mechanics).

Crack growth studies were conducted on soda lime silica, soda borosilicate and two binary soda silica glasses immersed in solutions of 1 Molar Li^+ , 1 Molar Cs^+ or deionized water at different pH values. A definite effect of the Li^+ and Cs^+ was observed on the V-K sub I curves in all but the soda lime glass. A plateau in crack velocity in the range 0.00000001 to 0.000000001 m/sec was measured on the binary soda-silica glasses for $K_{\text{sub I}} < 0.35 \text{ MPa m}^{1/2}$ power. These data are analyzed in terms of both the ion exchange and SiO_2 dissolution steps of the corrosion process. A model of crack growth in corrosive conditions is proposed.

500,822

PB85-195915

Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

Comparison of Failure Predictions by Strength and Fracture Mechanics.

Final rept.,

B. J. Pletka, and S. M. Wiederhorn. 1982, 22p

Pub. in Jnl. of Materials Science 17, n5 p1247-1268, 5 May 82.

Keywords: *Ceramics, *Failure, Strength, Predictions, Mechanical properties, Data, Stressing, Crack propagation, Confidence limits, Micro structure, Life(Durability), Reprints, Fracture mechanics.

Failure predictions for five ceramic materials were compared using fracture mechanics and strength techniques. Double torsion specimens were used to obtain the fracture mechanics data and stressing rate experiments were used to obtain the strength data. An error analysis based on the error propagation law was performed to determine confidence limits for the failure predictions. The implications of these results with regard to microstructural effects on crack propagation and design applications are discussed.

500,823

PB85-196053

Not available NTIS
National Bureau of Standards, Gaithersburg, MD.

Effect of Deformation on the Fracture of Si_3N_4 and Sialon.

Final rept.,

R. J. Fields, T. J. Chuang, E. R. Fuller, and N. J.

Tighe. 1983, 8p

Sponsored by North Atlantic Treaty Organization, Brussels (Belgium).

Pub. in Proceedings of the NATO Conference on Nitrogen Ceramics (2nd), Falmer, Sussex, England, July 27-August 7, 1981, p507-514 1983.

Keywords: *Silicon nitrides, Ceramics, Fracture properties, Creep properties, Toughness, Deformation, *Sialon, *Aluminum silicon oxynitride.

At high temperatures, ceramics can deform inelastically by time-dependent processes such as creep. The resulting strains are stress and time dependent, and must be added to the elastic strain to calculate the total strain. Whether or not it is appropriate to apply linear elastic fracture mechanics depends on the extent of the creep deformation zone relative to certain specimen dimensions. With this in mind, the loading-rate dependences of the fracture toughness of silicon nitride and various sialons were investigated at elevated temperatures. The resulting variations in toughness are explained in terms of possible micromechanisms of deformation and fracture. Schemes are presented for estimating the toughness in the case of small scale creep deformation and in the case of general creep deformation, in which the creep strain exceeds the elastic strain throughout the body.

500,824

PB85-202885

Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Inorganic Analytical Research Div.

Investigation of the Phase Transition in ZrTiO_4 and $\text{ZrTiO}_4\text{-SnO}_2$ Solid Solutions.

Final rept.,

A. E. McHale, and R. S. Roth. Feb 83, 3p

Pub. in Jnl. of the American Ceramic Society 66, n2 p18-20 Feb 83.

Keywords: *Tin oxides, *Solid solutions, *Phase transformations, *Crystal structure, X-ray diffraction, Titanium dioxide, Reprints, *Zirconium titanates.

A 'continuous' phase transition was found to occur in ZrTiO_4 , with a major discontinuity at 1125 plus or minus 10 degrees C. The space group of both forms of ZrTiO_4 is Pcnb . For specimens quenched from high temperatures, the volume of the unit cell was found to decrease linearly from about 1450 degrees C to the discontinuity with the major change occurring in the c-axis. The volume decreases considerably at this temperature and again continues to decrease with lower temperature annealing. The maximum unit cell dimensions in the high temperature structure are $a = 4.806$, $b = 5.035$, and $c = 5.498 \text{ \AA}$ with the minimum unit cell values of $a = 4.828$, $b = 5.035$ and $c = 5.348 \text{ \AA}$ in the low temperature form. Substitutional tin in solid solution was found to stabilize the high temperature structure type.

500,825

PB85-203396

Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Inorganic Materials Div.

Chevron-Notch Bend Testing in Glass: Some Experimental Problems.

Final rept.,

L. Chuck, E. R. Fuller, and S. W. Freiman. 1984, 8p

Contract DE-A105-80OR20679

Pub. in American Society for Testing and Materials Special Technical Publication 855, p167-175 1984.

Keywords: *Glass, Environments, Fracture strength, Flexing, Tests, Loads(Forces), Crack propagation, Brittleness, Reprints.

The study describes experimental difficulties in the use of the chevronnotch bend test to determine the plane-strain fracture toughness, for brittle materials. Four-point flexure tests were performed on soda-lime-silica glass and vitreous silica in both 'wet' and 'dry' environments and at various loading rates.

500,826

PB85-203404

Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Inorganic Materials Div.

Fatigue Properties of Ceramics with Natural and Controlled Flaws: A Study of Alumina.

Final rept.,

A. C. Gonzalez, H. Multhopp, R. F. Cook, B. R.

Lawn, and S. W. Freiman. 1984, 14p

Pub. in American Society for Testing and Materials Special Technical Publication 844, p43-56 1984.

Keywords: *Ceramics, *Fatigue(Materials), *Aluminum oxide, Strength, Defects, Stresses, Tests, Life(Durability), Loads(Forces), Predictions, Reprints.

A systematic study of the fatigue properties of an as-fired polycrystalline alumina containing either 'natural' (sawing damage) or indentation-induced (Vickers) strength-controlling flaws has been made. All fatigue strengths were measured in four-point bending in water. The study is presented in three steps: first, comparative Weibull analyses are made of inert strength data for the two flaw types, both to demonstrate the reduction in scatter that attends the indentation method and to characterize the flaw distributions for the as-sawn surfaces; next, fatigue data are taken on indented surfaces to determine relatively accurate fracture parameters for the alumina and to confirm that constant stressing rate tests can be used as a base for predicting the response in static loading; finally, the results from the two previous, independent steps are combined to generate lifetime responses for the surfaces with natural flaws, and fatigue data taken on such surfaces are used to evaluate these predictions.

500,827

PB85-205326

Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Inorganic Materials Div.

Subthreshold Indentation Flaws in the Study of Fatigue Properties of Ultrahigh-Strength Glass.

Final rept.,

T. P. Dabbs, C. J. Fairbanks, and B. R. Lawn. 1984,

12p

Sponsored by Office of Naval Research, Arlington, VA.

Pub. in American Society for Testing and Materials Special Technical Publication 844, p142-143 1984.

Keywords: *Defects, *Fatigue(Materials), *Glass, Crack propagation, Stresses, Failure, Strength, Fiber optics, Reprints.

The rate-dependent characteristics of subthreshold indentation flaws in glass are surveyed. In the first part, the kinetics of radial crack initiation within the indentation field are described. In the second part of the presentation, the fatigue properties of specimens with indentation flaws on either side of the threshold are discussed. Finally, the implications of the results concerning design criteria for the ultra-high strength domain of optical fibers are considered.

500,828

PB85-205904

Not available NTIS
National Bureau of Standards, Gaithersburg, MD.

Effects of Water and Other Dielectrics on Crack-Growth.

Final rept.,

S. M. Wiederhorn, S. W. Freiman, E. R. Fuller, and

C. J. Simmons. 1982, 19p

See also PB82-235896.

Pub. in Jnl. of Materials Science 17, n12 p3460-3478 1982.

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Keywords: *Alkali glass, *Crack propagation, Water, Dielectrics, Silica glass, Fractures(Materials), Reprints.

The effect of water and a variety of organic liquids on the crack growth rate in soda lime silica glass was investigated. When water is present in organic liquids, it is usually the principal agent that promotes subcritical crack growth in glass. In region I, subcritical crack growth is controlled primarily by the chemical potential of the water in the liquid; whereas in region II, crack growth is controlled by the concentration of water and the viscosity of the solution formed by the water and the organic liquid. In region III, where water does not affect crack growth, the slope of the crack growth curves can be correlated with the dielectric constant of the liquid. It is suggested that these latter results can be explained by electrostatic interactions between the environment and charges that form during the rupture of Si-O bonds.

500,829

PB85-207959

Not available NTIS

National Bureau of Standards, Gaithersburg, MD. Inorganic Materials Div.

Sharp vs. Blunt Crack Hypotheses in the Strength of Glass: A Critical Study Using Indentation Flaws.

Final rept.,

B. R. Lawn, K. Jakus, and A. C. Gonzalez. 1985, 10p. Sponsored by Office of Naval Research, Arlington, VA. Pub. in Jnl. of American Ceramic Society 68, n1 p25-34 1985.

Keywords: *Glass, Cracks, Strength, Defects, Indentation, Reprints.

The fundamental question as to whether the tip structure of brittle cracks is atomically sharp or has a rounded contour is examined in relation to current descriptions of strength-controlling flaws. The distinction between the two opposing viewpoints lies in the controlling flaw dimensions in the strength formulation; crack length in the first and tip radius in the second. Definitive evidence on the issue is obtained from aging tests on soda-lime glass, using indentations as controlled flaws.

500,830

PB85-222016

Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

High-Temperature Toughness of Silicon Carbide Materials in a Controlled Gaseous Environment.

Final rept.,

R. F. Krause, L. Chuck, and E. R. Fuller. 1982, 1p. Sponsored by Department of Energy, Washington, DC., Gas Research Inst., Chicago, IL., and Electric Power Research Inst., Palo Alto, CA.

Pub. in Proceedings of Annual Conf. on Materials for Coal Conversion and Utilization, Gaithersburg, MD., November 16-18, 1982, 159p.

Keywords: *Silicon carbides, Toughness, Controlled atmospheres.

The fracture toughness of three silicon carbide materials was measured in a controlled gaseous environment at elevated temperatures up to 1500C. Chevron-notched, four-point bend specimens were fractured at different displacement rates to obtain both a measure of fracture toughness and an indication of environmental crack growth and/or of crack-tip creep deformation. Experiments were conducted both in air and in a gaseous mixture of steam, carbon dioxide, sulfur dioxide, oxygen, and nitrogen thereby simulating the combustion of a producer gas.

500,831

PB85-222263

Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

Tectosilicates--New Data on Processing, Physical and Electronic Properties, and Chemical Durability.

Final rept.,

L. P. Cook, C. K. Chiang, and T. Hahn. 1982, 6p. Sponsored by Department of Energy, Washington, DC., Gas Research Inst., Chicago, IL., and Electric Power Research Inst., Palo Alto, CA.

Pub. in Proceedings of Annual Conf. on Materials for Coal Conversion and Utilization (7th), Gaithersburg, MD., November 16-18, 1982, p137-142.

Keywords: *Silicates, *Materials tests, Corrosion, Chemical attack, Ceramics, High temperature tests, Physical properties, Electronic properties, Durability, Magnetohydrodynamics, *Tectosilicates.

The extended abstract outlines the second of a series of papers aimed at defining the potential of the struc-

tural family of compounds known as the tectosilicates for MHD ceramic materials applications at moderate to high temperatures.

500,832

PB85-222297

Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

Reaction of Silicon Carbide with Product Gases of Coal Combustion.

Final rept.,

A. L. Dragoo, and J. L. Waring. 1982, 16p. Sponsored by Department of Energy, Washington, DC., Gas Research Inst., Chicago, IL., and Electric Power Research Inst., Palo Alto, CA.

Pub. in Proceedings of Annual Conf. on Materials for Coal Conversion and Utilization (7th), Gaithersburg, MD., November 16-18, 1982, p161-176.

Keywords: *Silicon carbides, *Materials tests, *Coal gasification, Ceramics, Nitridation, Oxidation, Chemical reactions.

The reactions of commercially manufactured silicon carbide ceramics--two materials without free silicon and two materials with free silicon('siliconized')--with air, N₂ + SO₂, and a simulated coal-combustion gas containing about seven volume percent O₂ were investigated. Samples were annealed in air and N₂ + SO₂ at 1400C for successive annealing times up to a total time of 12 hours. Samples were annealed in the simulated combustion gas at 1350C for four hours. For anneals in air and in simulated combustion gas, low cristobalite and, possibly, some tridymite were the main reaction products. The presence of SO₂ in N₂ appears to promote the nitridation of the silicon carbide ceramics.

500,833

PB85-222362

Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

Thermodynamic Activity and Vapor Pressure Models for Silicate Systems Including Coal Slags.

Final rept.,

J. W. Hastie, D. W. Bonnell, E. R. Plante, and W. S. Horton. 1982, 16p.

Sponsored by Department of Energy, Washington, DC., Gas Research Inst., Chicago, IL., and Electric Power Research Inst., Palo Alto, CA.

Pub. in Proceedings of Annual Conf. on Materials for Coal Conversion and Utilization (7th), Gaithersburg, MD., November 16-18, 1982, p265-280.

Keywords: *Thermodynamics, *Silicates, *Vapor pressure, *Mathematical models, High temperature tests, Experimental design, Comparison, Complex compounds, Ceramics, *Slags.

A new modeling approach is described for thermodynamic predictions of multicomponent, multiphase high temperature silicate systems including coal slags. The model, which attributes negative deviations from ideal solution behavior to the formation of complex liquids and solids, is demonstrated for quaternary systems containing K₂O, Al₂O₃, CaO, and SiO₂. Good agreement between the model predictions and experimental vapor pressure data is found.

500,834

PB85-227080

PC A05/MF A01

National Bureau of Standards, Gaithersburg, MD.

Inorganic Materials Div.

Computerized Fracture Mechanics Database for Oxide Glasses.

Technical note (Final),

S. W. Freiman, T. L. Baker, and J. B. Wachtman. Jun 85, 95p NBS/TN-1212

Also available from Supt. of Docs as SN003-003-02663-8. Prepared in cooperation with Rutgers - The State Univ., Piscataway, N.J. Center for Ceramics Research.

Keywords: *Fracture properties, *Glass, *Information systems, Oxides, Crack propagation, Modulus of elasticity, Chemical composition, Tables(Data), Ceramics, *Data bases, Computer applications.

Values of critical fracture toughness, fracture energy, subcritical crack growth exponents and Young's modulus, are compiled and tabulated for a wide variety of oxide glasses. A computerized data retrieval system has been formulated to allow for selection of data by either glass composition, investigator, or experimental technique, and year.

500,835

PB85-229318

Not available NTIS

National Bureau of Standards, Gaithersburg, MD. Polymers Div.

Elastic Constants of Two Dental Porcelains.

Final rept.,

H. R. Kase, J. A. Tesk, and E. D. Case. 1985, 9p

Pub. in Jnl. of Materials Science 20, p524-531 1985.

Keywords: *Dental materials, *Acid bonded reaction cements, *Determination of stress, *Porcelain, *Elastic properties, Temperature coefficient, Stress strain diagrams, Forecasting, Dynamic modulus of elasticity, Sonic tests, Reprints, *Ceramic metal seals, Numerical solution.

The development of stress that affects the bonding in porcelain-fused-to-metal (PFM) systems can be influenced by the temperature dependence of the elastic constants of both systems. Instead of using the normal, static procedure, e.g. determining the slope of a stress-strain curve, and measuring the lateral and vertical strains, in the study the sonic resonance technique was used to determine the elastic moduli for two dental body-porcelains. Young's and shear moduli for two dental porcelains obtained in the range from 20C (293 K) to 500C (773 K) are presented in the study. The data may in the future be used for refined stress calculations in PFM systems.

500,836

PB85-229987

Not available NTIS

National Bureau of Standards (NEL), Gaithersburg, MD. Thermophysics Div.

Comment on 'Measurement of Thermodynamic Parameters of Graphite by Pulsed-Laser Melting and Ion Channeling'.

Final rept.,

A. Cezairliyan. 1985, 2p

Pub. in Physical Review Letters 54, n11 p1208, 18 Mar 85.

Keywords: *Graphite, *Thermodynamic properties, Melting, Reprints, Laser applications, Ion channeling.

The work of Venkatesan et al. is briefly discussed and commented upon in light of similar research at the National Bureau of Standards.

500,837

PB85-230845

Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

Development of Potassium Aluminosilicate Ceramics for MHD (Magnetohydrodynamics) Application.

Final rept.,

L. P. Cook. 1981, 16p

Sponsored by Department of Energy, Washington, DC. Pub. in Proceedings of the Symposium on Engineering Aspects of Magnetohydrodynamics (19th), Tullahoma, Tennessee, June 15-17, 1982, p1-15 1981.

Keywords: *Silicate refractories, Ceramics, Magnetohydrodynamic generators, *Potassium aluminosilicates.

Refractory potassium aluminosilicate phases with reported melting points in excess of 1690C include KAlSi₂O₆, KAlSiO₄ and K(1+x)Al(1+x)Si(1+x)O₄. From a purely chemical standpoint these materials are expected to have substantial resistance to corrosion by MHD slag. A method for processing ceramics of these materials is being developed which results in densification without the use of additives. Using this method relatively well-sintered KAlSi₂O₆ ceramics (density 77-83% of theoretical) with moderate strength (35-45 MPa) have been produced.

500,838

PB86-110152

Not available NTIS

National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.

Crack Growth in Sialon.

Final rept.,

R. J. Fields, E. R. Fuller, T. J. Chuang, and L. Chuck. 1983, 11p

Sponsored by Army Research Office, Arlington, VA., National Science Foundation, Washington, DC., and Office of Naval Research, Arlington, VA.

Pub. in Proceedings of International Symposium on Fracture Mechanics of Ceramics (3rd), University Park, PA., Jul 15-17, 1981, Measurements, Transformations, and High Temperature Fracture, v6 p463-473 1983.

Keywords: *Crack propagation, *High temperature tests, *Bending stress, Fractures(Materials), Loads(Forces), *Sialon.

Field 11—MATERIALS

Group 11B—Ceramics, Refractories, and Glasses

An analysis of the bending of notched bars is presented for determining crack growth behavior directly from load-displacement records. The analysis is evaluated by experiments on glass bars in water. The analysis is then applied to the slow fracture of various sialon compositions. Micrographs of the resulting fracture surfaces are presented together with a discussion of a possible mechanism of crack growth in these materials.

500,839

PB86-136843

Not available NTIS

National Bureau of Standards, Gaithersburg, MD. Inorganic Materials Div.

Microstructure and Electrical Properties of Ceria-Based Ceramic Electrolytes.

Final rept.,

A. L. Dragoo, and C. K. Chiang. 1983, 14p

Pub. in Proceedings of Conference on High Temperature Solid Oxide Electrolytes, Upton, NY., August 16, 1983, v1 p268-281 1983.

Keywords: *Cerium dioxide, *Ceramics, *Electrical properties, *Electrolytes, Fuel cells, Molecular structure, Additives.

High-density, yttria- and gadolinia-doped ceria ceramics were found to exhibit notable differences in electrical properties which correlated with differences in the processing methods used to form the materials. Dopant concentrations of 8.5, 20 and 30 mol percent, with respect to cation concentration, were prepared. Three chemical processes were used to prepare well-mixed precursors which were calcined to oxide powders. Following forming and isostatic compaction, most samples were thermally sintered. Inhomogeneity impedance appeared to be influenced by calcination temperature, densification method, and dopant concentration. Microstructure examination and elemental analysis of samples by means of a scanning electron microscope (SEM) equipped with an analytical x-ray apparatus suggested A1 as a source of the different lattice impedance of the hot-pressed material and showed high Si concentrations associated with regions of large pores in gadolinia-doped materials.

11C. Coating, Colorants, and Finishes

500,840

PB85-172468

Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

Radiation Curing of Coatings.

Final rept.,

G. A. Senich, and R. E. Florin. 1984, 86p

Pub. in Jnl. of Macromolecular Science Review Macromol. Chem. Phys. C24, n2 p239-324 1984.

Keywords: *Coatings, *Curing, *Radiation effects, Industrial plants, Polymerization, Thermosetting resins, Plastics, Reprints.

The science and technology of curing organic materials with radiation is reviewed. Electron beam, ultraviolet, infrared, microwave, and high frequency radiation sources and the resin systems suitable for use with these sources are considered. Equipment necessary to affect a radiation cure is discussed and some practical problems unique to each radiation method are indicated. The application of radiation curing to industrial processes which employ inks and coatings is covered, with particular emphasis given to printing with radiation curable formulations. Included are discussions of the advantages and disadvantages of radiation curing inks, some typical ink components and formulations, the specialized machinery required, and the influence of parameters unique to radiation curing methods on the printing process. Other nonprinting but related industrial operations utilizing radiations for treating thin films and coatings are also considered. Some costs, examples, and market statistics are given for these commercial procedures. New nonconventional, but also nonradiation, alternative curing methods are discussed briefly. A bibliography of recommended further reading and a list of over two hundred fifty references are included.

500,841

PB85-196962

Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

Method for Preparing Cross-Sections of Films on Wear Surfaces for Transmission Electron Microscopy Study.

Final rept.,

L. K. Ives. 1983, 6p

Pub. in Wear 86, n1 p151-156, 1 Apr 83.

Keywords: *Protective coatings, Wear, Metal films, Coatings, Electron microscopy, Surfaces, Reprints.

A method for preparing cross sections for transmission electron microscopy study of surface layers which exist on bulk metal substrates is described. The surface layer or film is protected by a vacuum deposited or sputtered coating of a suitable metal. A mask is placed over the surface and non-masked areas are exposed to ion beam etching until the substrate is exposed. A subsequently applied thick electroplated layer adheres well to the ion etched substrate and seals the coated surface film against damage during slicing, grinding, etc. that are usual steps in preparation from bulk materials of thin foils for transmission electron microscopy study. The method was specifically developed for the analysis of boundary and extreme pressure lubrication films on wear surfaces. However, it is also applicable to the investigation of oxide, corrosion and other surface films.

500,842

PB85-205946

Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

Simple Model for the Numerical Simulation of Reflectance of Black Chrome Coating Systems.

Final rept.,

S. T. Wu, and L. W. Masters. 1984, 4p

Sponsored by Department of Energy, Washington, DC. Pub. in Jnl. of Coatings Technology 56, n711 p29-32 1984.

Keywords: *Coatings, Mathematical models, Reflectance, Reprints, *Black chrome, Solar collectors.

Black chrome has been used extensively as an absorptive coating in solar collector systems because of its high absorptance/emittance ratio as well as its general stable characteristics under various environmental conditions. This paper is to present a numerical simulation on the optical properties of black chrome coating systems. A simple model is developed based on the analytical studies as well as the experimental results. The black chrome coating is considered to be composed of three 'pseudo' layers. The dielectric constants of the material are determined with the mean field approach. Rouard's method is used for computing the reflectance spectra of the coating system. The model can be used to serve the engineering needs for correlating the optical performance with the properties of the material. A numerical example is provided to illustrate the approach.

500,843

PB86-102449

Not available NTIS

National Bureau of Standards (NEL), Gaithersburg, MD. Building Materials Div.

Selection of a Spatial Sampling Procedure for Evaluating the Defect Area of a Coated Steel Panel.

Final rept.,

D. P. Bentz, and J. W. Martin. Jul 85, 7p

Pub. in Jnl. of Coatings Technology 57, n726 p43-49 Jul 85.

Keywords: *Coatings, Evaluation, Defects, Sampling, Monte Carlo method, Reprints.

Various spatial sampling procedures for determining the defect area of a coated panel are assessed using Monte Carlo techniques. Spatial sampling procedures have many advantages over the comparative visual standards currently used in evaluating defect area. In a previous report, a full grid sampling procedure was employed; the primary disadvantage of this procedure was its long evaluation time. This procedure can be replaced by other sampling procedures with shorter sampling times as long as these other procedures are both accurate and easy to implement into actual practice. From the Monte Carlo simulations, systematic point sampling is found to be superior to both random point and stratified random point sampling in quickly estimating defect area proportion. Two other spatial sampling procedures may also find applications in coatings evaluation, linear sampling which effectively quantifies the corrosion area around a scribe mark and systematic area sampling which provides valuable information on the defect size distribution as well as the total defect area.

500,844

PB86-111416

Not available NTIS

National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.

SEM (Scanning Electron Microscope) Analysis of Clad-Ceramic Coatings after Hot Corrosion Testing.

Final rept.,

C. D. Olson. 1982, 2p

Sponsored by Electron Microscopy Society of America, Oak Ridge, TN.

Pub. in Proceedings of Annual Meeting on Electron Microscopy Society of America (40th), Washington, DC., August 9-13, 1982, p522-523.

Keywords: *Protective coatings, *Metals, *Corrosion prevention, *Ceramic coatings, *Scanning electron microscopy, *Energy dispersive X ray analysis, AISI 1015 steel.

Scanning electron microscope (SEM) and energy dispersive x-ray analysis (EDX) have been used to study protective coatings on metals under a hot corrosive gas environment. Coatings were arc plasma sprayed on AISI 1015 steel and evaluated as to corrosive characteristic and protection to the steel under the exposed environment.

500,845

PB86-113990

Not available NTIS

National Bureau of Standards, Gaithersburg, MD. Materials Chemistry Div.

New Technique to Study Corrosion Mechanisms under Organic Coatings.

Final rept.,

J. Kruger, and J. J. Ritter. 1982, 23p

Sponsored by American Chemical Society, Washington, DC.

Pub. in Proceedings of International Conference on Organic Coatings Science and Technology (8th), Athens, Greece, July 12-16, 1982 p383-405.

Keywords: *Polymer films, *Plastic coatings, *Corrosion prevention, *Iron, Electrochemistry, Ellipsometry, Protective coatings, pH, Procedures.

Transparent organic coatings on iron are used to simulate painted metal surfaces for simultaneous ellipsometric and electrochemical measurements. These studies show that significant changes occur both in the metal oxide film and in the subcoating environment during prolonged immersion in dilute Cl(-1) media. The relationship of these changes to aspects such as metal passivation, surface roughening, coating delamination, type of coatings, and inhibitor behavior are discussed.

500,846

PB86-138526

Not available NTIS

National Bureau of Standards, Gaithersburg, MD. Polymer Science and Standards Div.

Mechanical Properties of Compliant Coating Materials.

Final rept.,

D. L. Hunston, C. Yu, and G. W. Bullman. 1984, 5p

Sponsored by Office of Naval Research, Arlington, VA. Pub. in Proceedings of Energy Sources Technology Conference - Laminar Turbulent Boundary Layer, New Orleans, Louisiana, February 12-16, 1984 p85-89.

Keywords: *Coatings, Mechanical properties, Viscoelasticity, Turbulent flow, Synthetic elastomers, Polyvinyl chloride, Acrylonitrile copolymers, Diene resins.

Analyzing and understanding the interactions that occur at the interface between a compliant surface coating and a fluid undergoing turbulent flow requires a detailed knowledge of the mechanical properties of the coating material. The present work involves a comprehensive characterization of the shear viscoelastic properties of coating materials. A nitrile rubber is used to examine the general types of behavior expected for coatings.

500,847

PB86-142908

Not available NTIS

National Bureau of Standards (NEL), Gaithersburg, MD. Building Materials Div.

Reflection/Absorption Fourier Transform Infrared Spectroscopy Studies of the Degradation of Organic Protective Coatings on Steel.

Final rept.,
T. Nguyen, and W. E. Byrd. 1985, 6p
Pub. in Proceedings of the American Chemical Society, Polymeric Materials Science and Engineering, Chicago, Illinois, September 7-12, 1985, v53 p568-573.

Keywords: *Protective coatings, *Steels, *Corrosion, *Degradation, Absorption, Polybutadiene, Reflection, Complex compounds, Oxidation, Infrared spectroscopy, *Fourier transform spectroscopy.

The application of FTIR-RA for studying the degradation, resulting from exposure to a 40C and 82% RH environment, of two types of organic coatings on cold-rolled steel is presented in the paper. FTIR-RA results indicate bond weakening in the polymer, dehydration and bond scissions at the aryl-isopropylidene group of amine-cured epoxy coatings on cold-rolled steel. On the other hand, the polybutadiene coating on steel specimens show, not only bond weakening both within the coating and at the interface, but also extensive corrosive-related degradation which results in the formation of various highly oxidized products and losses in unsaturation. The characterization of fairly complex organic molecules formed during the oxidation and degradation by FTIR-RA offers a powerful means for studies of the degradation processes, both in the bulk and at the interface of protective coatings on steel subjected to corrosive environments.

500,848
PB86-142916 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Building Materials Div.

Reflection/Absorption Fourier Transform Infrared Spectroscopy of the Degradation of Protective Coatings on Mild Steel.

Final rept.,
T. Nguyen, and W. E. Byrd. 1985, 18p
Pub. in Proceedings of the International Conference on Organic Coatings Science and Technology (11th), Athens, Greece, July 8-12, 1985, p235-252.

Keywords: *Protective coatings, *Steels, *Corrosion, *Degradation, Absorption, Polybutadiene, Reflection, Complex compounds, Oxidation, Infrared spectroscopy, *Fourier transform spectroscopy.

The application of reflection/absorption Fourier transform infrared spectroscopy (FTIR-RA) for studying the degradation of two types of coating on steel after exposure to 40C/80% RH environments is presented in the paper. FTIR-RA results indicate the occurrence of (1) bond weakening in the polymer film, (2) dehydration and (3) bond scissions at the isopropylidene group of amine-cured after exposure to 40C and 80% RH environments for 7 months. On the other hand, the polybutadiene coating specimens show, not only bond weakening but also extensive degradation which results in the formation of various oxidized products and losses in unsaturation. The characterization of complex molecules that are formed during the oxidation and degradation by FTIR-RA offers a powerful means for studies of the degradation processes, both in the bulk and at the interface of protective coatings on steel.

11D. Composite Materials

500,849
PB85-182897 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.

Abrasive Wear of Aluminum Matrix Composites.

Final rept.,
K. J. Bhansali, and R. Mehrabian. 1982, 5p
Pub. in Jnl. of Metals 34, n9 p30-34 1982.

Keywords: *Wear, Composite materials, Aluminum oxide, Silicon carbides, Abrasion, Reprints, *Aluminum matrix composites.

Abrasive wear resistance of aluminum matrix composites containing Al₂O₃ and SiC was investigated using a dry sand/rubber wheel abrasion tester. Composites containing Al₂O₃ were found to be superior to those containing SiC. This behavior was attributed to the formation of a brittle bond at the interface between aluminum matrix and SiC. Wear resistance of a composite containing large 142 micrometers Al₂O₃ was better

than that of composites containing smaller Al₂O₃ particles, and was comparable to AISI 1345 steel heat treated to a hardness of 67 HRC.

500,850
PB85-196194 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.

Erosion of Ceramic Materials: The Role of Plastic Flow.

B. J. Hockey, and S. M. Wiederhorn. 1979, 27p
Pub. in Proceedings of International Conference on Erosion by Liquid and Solid Impact (5th), Cambridge, England, September 3-6, 1979, p1-26.

Keywords: *Ceramics, *Erosion, Wear, Aluminum oxide, Plastic flow, Glass, Silicon carbide, Magnesium oxides.

Plastic flow has been shown recently to play a crucial role in the erosive wear of ceramic materials that are brittle at room temperature. In this paper, evidence for plastic flow during the erosion of brittle solids by solid particles is reviewed and discussed. Evidence for plastic flow comes from three sources: optical and scanning electron microscopy studies of single particle impact sites; investigations of erosion rate as a function of impact angle; and investigations of impact sites by transmission electron microscopy. This discussion of plastic flow will include an evaluation of several recent theories developed to explain the erosion of ceramic materials. The importance of dynamic values of both the hardness and the critical stress intensity factor to the erosion process is emphasized.

500,851
PB85-205912 Not available NTIS
National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.

Stiffness and Internal Stresses of Woven-Fabric Composites at Low Temperatures.

Final rept.,
R. D. Kriz. 1984, 7p
Sponsored by Department of Energy, Washington, DC. Office of Fusion Energy.
Pub. in Advances in Cryogenic Engineering Materials 30, p1-7 1984.

Keywords: *Woven fiber composites, Cryogenics, Stiffness, Residual stress, Reprints.

Woven-fabric composites are used in superconducting magnets and in containment of cryogenic liquids. Here, the mechanical response of a plain-weave laminated composite at cryogenic temperatures is studied by predicting the load-deformation response of a fundamental 'unit cell.' At present, only tensile loads are studied in the warp direction. Results show that stresses normal to the warp-fill interface increase with increasing warp angle; the largest effect occurs in the matrix region. Thermal loads increase these stresses in the matrix region and decrease these stresses in the fill region. Stiffness increases with decreasing warp angle.

500,852
PB85-205920 Not available NTIS
National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.

Influence of Ply Cracks on Fracture Strength of Graphite/Epoxy Laminates at 76 K.

Final rept.,
R. D. Kriz. 1984, 16p
Sponsored by National Research Council, Washington, DC and Department of Energy, Washington, DC. Office of Fusion Energy.
Pub. in American Society for Testing and Materials, Special Technical Publication 836, p250-265 1984.

Keywords: *Epoxy laminates, Fracture strength, Cryogenics, Oriented fiber composites, Reprints, Carbon fiber reinforced plastics, Epoxy matrix composites, Graphite reinforced composites, Cracks, Finite element analysis.

Quasi-isotropic laminates were fabricated from graphite/epoxy and quasi-statically loaded in tension at 76 K until fracture occurred. Fibers in 0-deg plies carry the largest portion of the tensile load; the weaker 90- and 45-deg plies crack at loads much lower than fracture strength. The effect of ply cracks on fracture of load-bearing 0-deg plies was examined to understand how defects affect laminate strength. A generalized plane-strain finite-element model was used to predict stress gradients in the 0-deg ply near the crack tip. Variations in residual stress caused by changes in temperature and absorbed moisture were included in the analysis.

500,853
PB85-207330 Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.

Elastic Constants of an Anisotropic, Nonhomogeneous Particle-Reinforced Composite.

Final rept.,
H. M. Ledbetter, S. K. Datta, and R. D. Kriz. 1984, 7p
Sponsored by Defense Advanced Research Projects Agency, Arlington, VA.
Pub. in Acta Metallurgica 32, n12 p2225-2231 1984.

Keywords: *Particulate composites, Single crystals, Silicon carbides, Elastic properties, Reprints, Aluminum matrix composites.

Experimentally and theoretically, we studied the elastic constants of a particle-reinforced-composite wrought plate produced by powder-metallurgy methods. The particles, 30% by volume, consisted of single crystals of alpha-SiC with sizes near 5 micrometers. The matrix consisted of 6061 Al alloy with original sizes up to 20 micrometers. By measuring ultrasonic-wave velocities using a pulse-echo method, we determined the complete nine-component elastic-constant tensor. Thermal-mechanical processing introduced orthotropic macroscopic elastic symmetry into the material. Besides the Voigt elastic constants, we report all the usual engineering elastic constants: Young moduli, shear moduli, Poisson ratios, and bulk modulus (reciprocal compressibility). The elastic stiffnesses show large negative departures from a rule-of-mixture: up to 42%. Large elastic anisotropies also occur: 13% in Young's modulus, 12% in shear modulus, and 13% in Poisson's ratio. Explanation of these physical-property peculiarities lies in the microstructure. SiC particles are distributed nonhomogeneously. With Al, they form an enriched 'sea' that surrounds 'islands' of Al. These nonspherical islands are aligned and produce anisotropy. Using wave-scattering methods and ensemble averaging, we develop a theory that predicts all the observed physical-property phenomena.

500,854
PB85-207991 Not available NTIS
National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.

Damping Metal-Matrix Composites: Measurement and Modeling.

Final rept.,
H. M. Ledbetter, and S. K. Datta. Nov 84, 18p
Pub. in Proceedings of Vibration Damping Workshop, Long Beach, CA., February 27-29, 1984, pW-1-W-18.

Keywords: Composite materials, Damping, Elastic properties, Internal friction, Measurement Mathematical models, *Metal matrix composites.

Both experimentally and theoretically, the authors consider attenuation of elastic waves in a composite consisting of elastic reinforcing particles dispersed in an elastic matrix. The authors consider only geometrical attenuation caused by scattering from particles. The authors model contains the effects of particle volume fraction, particle shape, particle size, particle elastic constants, matrix elastic constants, measurement frequency, and elastic-wave polarization.

500,855
PB86-107430 PC A03/MF A01
National Bureau of Standards (NML), Gaithersburg, MD. Office of Standard Reference Materials.

Glass Fiberboard SRM (Standard Reference Materials) for Thermal Resistance.

Final rept.,
J. G. Hust. Aug 85, 35p NBS/SP-260/98
Also available from Supt. of Docs as SN003-003-02674-3. Library of Congress catalog card no. 85-600566.

Keywords: *Thermal conductivity, *Fiberboards, *Heat resistant materials, *Glass particle composites, Standards, Temperature, Density(Mass/volume), Comparison, Insulation, *Standard reference materials, Certified reference materials.

The apparent thermal conductivity data that provided the basis for the certification of glass fiberboard as an SRM of thermal resistance are reported and analyzed. New data for the extension of the temperature range of this SRM to 100 K are included. Detailed analysis and intercomparisons of previously described NBS and other published data are given. These data are represented by an equation describing the dependen-

Field 11—MATERIALS

Group 11D—Composite Materials

cies of the data on temperature and density. Certified values of thermal resistance are given for temperatures from 100 to 300 K and densities from 113 to 145 kg/cm³.

500,856

PB86-111812

Not available NTIS

National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.

Monitoring Elastic Stiffness Degradation in Graphite/Epoxy Composites.

Final rept.,

R. D. Kriz, 1982, 5p

Sponsored by American Society for Nondestructive Testing, Columbus, OH.

Pub. in Proceedings of American Society for Nondestructive Testing Conference, Boston, MA., March 22-25 and Pittsburgh, PA., October 4-7, 1982, p160-164.

Keywords: *Graphite composites, *Epoxy resins, *Stiffness methods, Composite materials, Elastic analysis, Degradation, Moisture, Nondestructive testing.

Stiffness-critical design utilizes the high elastic moduli of graphite/epoxy composites. Elastic-stiffness degradation is therefore important. Here, we describe a non-destructive technique that measures the degree of degradation of the fiber or matrix stiffness. This technique monitors an acoustic beam's propagation direction, which depends on the composite's degree of elastic anisotropy. The epoxy-matrix used in this study is a commonly produced TGDDM-DDS epoxy resin that was saturated with absorbed moisture. The fiber experiment verified that the moisture degradation of the epoxy elastic stiffness altered the elastic anisotropy; the direction of the acoustic beam changed 5 degrees. The authors consider also the effect of fiber-stiffness degradation on the direction of propagation.

500,857

PB86-119476

Not available NTIS

National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.

Influence of Damage on Mechanical Properties of Woven Composites at Low Temperatures.

Final rept.,

R. D. Kriz, 1985, 4p

Sponsored by Department of Energy, Washington, DC. Office of Fusion Energy.

Pub. in Jnl. of Composites Technology and Research 7, n2 p55-58 1985.

Keywords: *Mechanical properties, *Composite materials, *Woven fiber composites, *Damage, Low temperature tests, Stress strain diagrams, Laminates, Reinforced plastics, Modulus of rupture tests, Reprints.

Large quantities of nonmetallic woven composites will be used in magnetic fusion energy structures at low temperatures. The authors predicted and measured the influence of crack formation on the mechanical performance of standard glass/epoxy laminates (G-10CR, G-11CR) at low temperatures. From experiments with tension loads, the authors studied the formation of damage as a collection of fiber breaks, fiber bundle cracks, and delaminations between adjacent fiber bundles. The authors measured fiber bundle cracks in the laminate interior and individual fiber fracture at the laminate edges. They discovered that the sequence and type of damage control the discontinuities ('knee') in the load-deformation (stress-strain) diagrams. The authors found that G-11CR has two knees and three distinct moduli, whereas G-10CR has only two moduli and a single knee at a lower strain than G-11CR. Decrease in moduli measured near the knees compared well with predictions from the finite element model.

500,858

PB86-122769

Not available NTIS

National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.

Physical-Property Modeling in Silicon-Carbide/Aluminum.

Final rept.,

H. M. Ledbetter, S. K. Datta, R. D. Kriz, and M. W.

Austin, 1984, 27p

Sponsored by Defense Advanced Research Projects Agency, Arlington, VA.

Pub. in Proceedings of Annual Discontinuous Reinforced Aluminum Composites Working Group Meeting (6th), Park City, Utah, January 4-6, 1984, p69-95.

Keywords: *Composite materials, *Physical properties, *Metal matrix composite, *Aluminum, *Silicon

carbide, Elastic properties, Specific heat, Thermal expansion, Internal friction.

The authors review recent NBS studies, experimental, and theoretical, on physical properties of particle-reinforced metal-matrix composites. They focus on silicon-carbide/aluminum and consider four physical properties: elastic constants, thermal expansivity, specific heat, and internal friction.

500,859

PB86-138427

Not available NTIS

National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.

Elastic Representation Surfaces of Unidirectional Graphite/Epoxy Composites.

Final rept.,

R. D. Kriz, and H. M. Ledbetter, 1985, 15p

Sponsored by Department of Energy, Washington, DC. Pub. in Proceedings of Recent Advances in Composites in the United States and Japan, Hampton, Virginia, June 1983, ASTM STP 864, p661-675 1985.

Keywords: *Oriented fiber composites, Elastic properties, Carbon fiber reinforced plastics, Epoxy matrix composites, Graphite reinforced composites.

Unidirectional graphite/epoxy composites exhibit high elastic anisotropy and unusual geometrical features in their elastic-property polar diagrams. From the five-component transverse-isotropic elastic-stiffness tensor we compute and display representation surfaces for Young's modulus, torsional modulus, linear compressibility, and Poisson's ratios. Based on Christoffel-equation solutions, we describe some unusual elastic-wave-surface topological features. Musgrave considered in detail the differences between phase-velocity and group-velocity surfaces arising from high elastic anisotropy. For these composites, we find effects similar to, but more dramatic than, Musgrave's. Some new, unexpected results for graphite/epoxy include: a shearwave velocity that exceeds a longitudinal-wave velocity in the plane transverse to the fiber; a wave that changes polarization character from longitudinal to transverse as the propagation direction sweeps from the fiber axis to the perpendicular axis.

500,860

PB86-138518

Not available NTIS

National Bureau of Standards, Gaithersburg, MD. Polymer Science and Standards Div.

Effects of Lay-up, Temperature, and Loading Rate in Double Cantilever Beam Tests of Interlaminar Crack Growth.

Final rept.,

D. L. Hunston, and W. D. Bascom, 1983, 2p

Pub. in Composites Technology Review 5, n4 p118-119 1983.

Keywords: *Composite materials, *Delaminating, Crack propagation, Temperature, Loading rate, Cantilever beams, Tests, Reprints.

The problem of delamination in composites has led to an interest in techniques for studying interlaminar crack growth. The double cantilever beam specimen is a major tool in this area. In an effort to help establish this test as a more quantitative technique, the variables of ply orientation, test temperature, and loading rate were examined. In selecting the lay-up pattern for the specimen, it was found that control of the crack path, specimen symmetry, and specimen stiffness were important considerations. In performing such experiments, the test temperature and loading rate were found to have relatively little effect with brittle matrix resins.

11E. Fibers and Textiles

500,861

PB85-197549

Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

Flame Retardation of Cellulose By Thiocyanates. Preliminary Study.

Final rept.,

R. J. McCarter, 1981, 12p

Pub. in Jnl. of Fire Retardant Chemistry 8, n3 p157-168 Aug 81.

Keywords: *Fire resistant materials, *Insulation, *Cellulose, *Combustion inhibitors, Sodium thiocyanates,

Safety, Potassium thiocyanates, Newsprint, Fibers, Reprints.

Sodium and potassium thiocyanate were found effective flame retardants for cellulose at addition levels circa 1 1/2 weight percent. The properties of these deliquescent salts permit their interstitial deposition in newsprint fibers with a minimal amount of aqueous solvent and suggest their possible utility for retarding cellulosic loose-fill insulation. Samples of such insulation were prepared in laboratory-scale equipment, using the thiocyanates in combination with other required inhibitors of smoldering and corrosion. Combustion tests of these samples were found to approximate the requirements of federal safety standards for such insulation. Thermal analysis is reported of the effects of various retardants upon the pyrolysis of cellulose and newsprint fibers.

500,862

PB86-166642

PC A06/MF A01

National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.

Fire Behavior of Upholstered Furniture.

Final rept.,

V. Babrauskas, and J. Krasny, Nov 85, 106p NBS/

MONO-173

Also available from Supt. of Docs as SN003-003-02710-3. Library of Congress catalog card no. 85-600620.

Keywords: *Furniture, *Upholstery, *Fire tests, *Flammability, Ignition, Smoke, Flame propagation, Heat flux.

A systematic review is made of engineering data on the major aspects of upholstered furniture flammability: cigarette ignition, small open flame ignition, radiant ignition, transition from smoldering to flaming, flame spread rates, and heat release and mass loss rates during fully-involved burning. Other areas discussed, but for which less data are available, include smoke production and radiant heat fluxes. Mattresses and transportation vehicle seating are included, along with upholstered chairs, loveseats, and sofas. Appropriate test methods most suitable for measuring each of these properties are discussed. Where available, relationships are presented which permit the quantitative prediction of full-scale furniture behavior from bench-scale tests. Where such relationships are not available, generalizations of qualitative results of empirical tests are given. Areas where substantive work is not available are outlined.

11F. Metallurgy and Metallography

500,863

PATENT-4 538 671

Not available NTIS

Department of Commerce, Washington, DC.

Arc Furnace for the Production of Small Investment Castings of Reactive or Refractory Metals Such as Titanium.

Patent,

R. M. Waterstrat. Filed 7 Feb 84, patented 3 Sep 85,

8p PB86-137247, PAT-APPL-6-577 855

Sponsored by American Dental Association Health Foundation, Washington, DC.

This Government-owned invention available for U.S. licensing and, possibly, for foreign licensing. Copy of patent available Commissioner of Patents, Washington, DC 20231 \$1.00.

Keywords: *Electric arc furnaces, *Patents, *Investment casting, Titanium, Chemical reactivity, Casting, PAT-CL-164-514.

An arc furnace and investment casting apparatus includes a copper base with an integrally formed crucible having a passage therethrough. A vacuum chamber is positioned on the top of the copper crucible with a non-consumable cathode projecting into the chamber to effect melting of metal placed in the crucible. A vacuum chamber is also suspended beneath the crucible for support of a mold to receive molten metal flowing through the passage.

500,864

PB85-172484

Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

Thermosolutal Convection during Directional Solidification.

Final rept.,
G. B. McFadden, R. G. Rehm, S. R. Coriell, W. Chuck, and K. A. Morrish. Dec 84, 13p
Pub. in Metallurgical Transactions 15A, p2125-2137 Dec 84.

Keywords: *Convection, *Solidification, Prandtl number, Nonlinear differential equations, Diffusion, Temperature, Concentration(Composition), Fluid flow, Velocity, Schmidt number, Reprints, *Binary alloys.

During solidification of a binary alloy at constant velocity vertically upwards, thermosolutal convection can occur if the solute rejected at the crystal-melt decreases the density of the melt. The authors assume that the crystal-melt interface remains planar and that the flow field is periodic in the horizontal direction. The time-dependent nonlinear differential equations for fluid flow, concentration, and temperature are solved numerically in two spatial dimensions for small Prandtl numbers and moderately large Schmidt numbers. For slow solidification velocities, the thermal field has an important stabilizing influence: near the onset of instability the flow is confined to the vicinity of the crystal-melt interface. For fixed velocity as the concentration increases, the horizontal wavelength of the flow decreases rapidly; a phenomena also indicated by linear stability analysis. The lateral inhomogeneity in solute concentration due to convection is obtained from the calculations. For a narrow range of solutal Rayleigh numbers and wavelengths, the flow is periodic in time.

500,865

PB85-172492

Not available NTIS

National Bureau of Standards, Gaithersburg, MD.
Nonplanar Interface Morphologies during Unidirectional Solidification of a Binary Alloy.

Final rept.,
G. B. McFadden, and S. R. Coriell. Jul 84, 9p
Sponsored by Defense Advanced Research Projects Agency, Arlington, VA.
Pub. in Physica 12D, n1-3 p253-261 Jul 84.

Keywords: *Solidification, Interfaces, Morphology, Reprints, *Binary alloys.

During directional solidification of a binary alloy, a planar solidification interface may become unstable and develop into a cellular nonplanar interface, exhibiting periodic structure transverse to the growth direction. Steady state two-dimensional temperature, solute concentration, and interface shapes are calculated numerically and the solute inhomogeneity (microsegregation) in the solidified material obtained. Specific results are presented for an aluminum alloy containing silver for solidification velocities of 0.01 and 1.0 cm/s, which corresponds to the constitutional supercooling and absolute stability regimes, respectively.

500,866

PB85-182798

Not available NTIS

National Bureau of Standards, Gaithersburg, MD.
Studies of the Friction Transients During Break-In of Sliding Metals.

Final rept.,
P. J. Blau. 1981, 9p
Pub. in Proceedings of Leeds-Lyons Conference on Running-In Process in Tribology (8th), Lyon, France, September 8-11, 1981 p175-183 1982.

Keywords: *Friction, *Copper alloys, *Aluminum alloys, Steels, Friction tests, Microstructure, Wear, Sliding friction, Copper alloy 15Ag, Aluminum alloy 4.5Cu 17Si.

A ball-on-flat, stroke-by-stroke friction tester (tribometer) was used to study the initial friction changes which occurred when 52100 steel balls were slid unlubricated on several alloys: Cu-15wt%Ag, Al-17wt%Si-4.5wt%Cu, and a dual phase steel with 0.14wt%C-1.56wt%Mn-0.63Si and rare earth additions. Computer test control, recording of data, and plotting of data aided analysis of various break-in effects on friction coefficient: air versus Argon environments, surface finishes, and applied loads. Differences in the properties of the tested materials and their microstructures were used to interpret the differences in their sliding friction behavior. The shapes of friction coefficient versus number of stroke plots were used in these interpretations.

500,867

PB85-182822

Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

Phase Diagram Features Associated with Multicritical Points in Alloy Systems.

Final rept.,
S. M. Allen, and J. W. Cahn. 1983, 16p
Grant NSF-DMR80-22277
Sponsored by American Society for Metals, Metals Park, OH., and Materials Research Society, University Park, PA.
Pub. in Proceedings of a Symposium on Alloy Phase Diagrams, Boston, MA, November 1982, Materials Research Society Symposia Proceedings, v19 p195-210 1983.

Keywords: *Phase diagrams, *Critical point, *Alloys, Binary systems(Materials).

Many features in the vicinity of critical points in phase diagrams can be illustrated using a Landau type free energy expansion as a power series in one or more order parameters and composition. This simple approach can be used with any solution model. It also predicts limits to metastability, and is useful for understanding mechanisms of phase change. The theory is applied to all the critical points that can occur in binary systems according to a Landau theory: critical consolute points order-disorder transition, tricritical points, critical end points, as well as to systems in which two transitions such as chemical and magnetic ordering occur.

500,868

PB85-183283

Not available NTIS

National Bureau of Standards (NEL), Gaithersburg, MD. Mathematical Analysis Div.

Morphological Stability in the Presence of Fluid Flow in the Melt.

Final rept.,
G. B. McFadden, S. R. Coriell, R. F. Boisvert, M. E. Glicksman, and Q. T. Fang. Dec 84, 8p
Pub. in Metallurgical Transactions A, 15A p2117-2124 Dec 84.

Keywords: *Melting, *Fluid flow, Stability, Morphology, Hydrodynamics, Reprints.

Recent experiments have shown that the presence of a vertical buoyancy-driven flow adjacent to an initially cylindrical crystal-melt interface may produce a time-dependent helical deformation of the interface, with a rotation period ranging from several minutes to many hours, depending upon the width of the melt. The temperature distribution is such that the interface is expected to be morphologically stable in the absence of fluid flow. A linear stability analysis reveals that the instability is due to a coupling between a basic hydrodynamic boundary separating the two phases. The crystal-melt interface lowers the critical Grashof number of an analogous rigid-walled system by an order of magnitude for succinonitrile with a Prandtl number $P=22.8$; furthermore, the hydrodynamic mode that is actually destabilized by the interface is not the least stable mode in the rigid-walled system for $P=22.8$. The results show that the instability may be regarded either as a rather large alteration of a basic hydrodynamic instability by the crystal-melt interface, or as a significant modification of the morphological stability of the interface by the presence of the buoyant flow.

500,869

PB85-184539

Not available NTIS

National Bureau of Standards, Gaithersburg, MD.
Diffusion-Induced Grain Boundary Migration.

Final rept.,
D. B. Butrymowicz, J. W. Cahn, J. R. Manning, D. E. Newbury, and T. J. Piccone. 1983, 11p
Sponsored by American Ceramic Society, Columbus, OH.
Pub. in Proceedings of a Special Conference of the Annual Meeting of the American Ceramic Society (84th), Cincinnati, OH., May 4-5, 1982, Advances in Ceramics, v6 p202-212 1983.

Keywords: *Grain boundaries, *Diffusion, Migration, Ceramics, Metals, Kirkendall effect.

The diffusion of a solute into or out of polycrystalline materials at temperatures at which only grain boundary diffusion is significant has been observed to induce grain boundaries to migrate in a large number of binary metal systems. This unexpected grain boundary migration leads to vastly enhanced mass transport and leaves altered concentrations of solute atoms in the regions traversed by the boundary. Recently suggested mechanisms for this effect depending on a grain boundary Kirkendall effect may explain why it has not yet been observed in ceramic systems.

500,870

PB85-184620

Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

Rate Effects in Hardness.

Final rept.,
C. J. Fairbanks, R. S. Polvani, S. M. Wiederhorn, B. J. Hockey, and B. R. Lawn. 1982, 3p
Pub. in Jnl. Mater. Sci. Lett. 1, n9 p391-393 Sep 82.

Keywords: *Hardness, Copper, Tungsten, Glass, Indentation, Deformation, Kinetics, Reprints.

Some preliminary results showing rate effects in the hardness of selected materials are reported. Copper, tungsten and soda-lime glass all show a decline in hardness with duration of contact. The observations offer a new avenue for studying deformation processes in materials.

500,871

PB85-184646

Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

Monitoring the Sliding Contact Conditions in Laboratory Wear Tests of Metals Using Time-Dependent Variations in Friction Coefficients.

Final rept.,
P. J. Blau. 1982, 10p
Pub. in Proceedings of Conference on Time-Dependent Failure Mechanisms and Assessment Methodologies, Gaithersburg, MD, April 20-22, 1982, p145-154.

Keywords: *Wear, Friction, Metals, Monitoring, Wear tests, Reprints.

The concept of monitoring sliding conditions by observing changes in friction coefficient (i.e. friction forces) may lead to improved reproducibility in laboratory testing as well as to a better knowledge of basic sliding processes. This approach involves the identification and characterization of friction coefficient versus time (or cycles, or distance) curves. It also involves detailed microscopy of metal sliding contact surfaces which have been subjected to dry wear conditions. Systematic analysis of data for various metals and alloys sliding under similar controlled conditions has shown quite different running-in behavior. The balance of dominant wear processes was seen to influence the friction curve 'signatures'. Several examples of friction coefficient variation analysis for dry sliding of metals will be given.

500,872

PB85-187383

Not available NTIS

National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.

Elastic-Constant Anomalies at the Neel Transition in Fe-18Cr-3Ni-12Mn.

Final rept.,
H. M. Ledbetter, and E. W. Collings. 1985, 5p
Sponsored by Defense Department, Canberra (Australia).
Pub. in Materials Science and Engineering 68, p233-237 1985.

Keywords: *Elastic properties, Austenitic stainless steels, Neel temperature, Ultrasonic tests, Cryogenics, Reprints, *Steel 18Cr 12Mn 3Ni, Magnetic susceptibility.

The elastic constants of an 18Cr-3Ni-12Mn austenitic stainless steel (where the steel composition is given in approximate weight per cent) were measured ultrasonically between room temperature and liquid helium temperature. All the elastic constants change anomalously and reversibly near 191 K, which magnetic susceptibility measurements show to be the Neel (paramagnetic-to-antiferromagnetic) transition temperature.

500,873

PB85-187748

Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

Surface Melting of an Alloy Under Steady State Conditions.

Final rept.,
J. A. Sekhar, R. Mehrabian, and H. L. Fraser. 1981, 13p
Sponsored by Metallurgical Society of AIME, Warrendale, PA.
Pub. in Proceedings of Symposium AIME Annu. Meet. Lasers in Metallurgy (110th), Chicago, IL, February 22-26, 1981, p207-219.

Field 11—MATERIALS

Group 11F—Metallurgy and Metallography

Keywords: *Melting, *Aluminum alloys, Steady state, Heat transmission, Aluminum alloy 4.5Cu, Rapid solidification.

A combined theoretical and experimental study is described for the surface melting of an Al-4.5 wt% Cu alloy substrate subjected to a high intensity stationary heat flux. Both the calculations and the experiments were done under steady state conditions. That is, the heat flux absorbed, through the circular region on the bounding surface of the substrate, is exactly balanced by conduction of heat into the substrate - thermal profiles remain the same after an initial transient. The heat flow model is based on a new formulation and solution methodology of the heat flow equation for the two free moving boundary problem at hand. The experiments were carried out on an electron beam welding apparatus especially modified for rapid solidification studies. Agreement between theory and experiment is shown to be reasonably good considering the limitations of the former due to a number of assumptions.

500,874

PB85-187755

Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

Morphological Stability of Electron Beam Melted Aluminum Alloys.

Final rept.,

R. J. Schaefer, S. R. Coriell, R. Mehrabian, C.

Fenimore, and F. S. Biancaneillo. 1982, 11p

Sponsored by Office of Naval Research, Arlington, VA. Pub. in Proceedings of Symposium on Rapidly Solidified Amorphous and Crystalline Alloys, Boston, MA, November 16-19, 1981, v8, p79-89 1982.

Keywords: *Aluminum alloys, Stability, Solidification, Melting, Rapid solidification.

For constant velocity solidification, morphological stability theory delineates the temperature gradients required for plane front solidification of a specific alloy. Using electron beams, surface heating of metals can be carried out with sufficiently well characterized thermal input to permit reliable use of computer models of melting and solidification. From numerical calculations, the growth velocity and temperature gradients as a function of position during resolidification can be obtained; combining these results with (constant velocity) morphological stability theory indicates the resolidification regimes for which the plane front is unstable. Presumably, completely planar solidification may be attained by selecting heating modes such that the region of instability is totally avoided, but the expected interface morphology is more difficult to predict if the interface passes briefly through an unstable region and then re-enters a region of stability. Aluminum-silver and aluminum-manganese alloys were melted under an electron beam with particular emphasis on attaining solidification sufficiently rapidly to satisfy the gradient-independent absolute stability condition.

500,875

PB85-195972

Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

Characterization of Wear Surfaces and Wear Debris.

Final rept.,

A. W. Ruff, L. K. Ives, and W. A. Glaeser. 1981, 55p

Sponsored by American Society for Metals, Metals Park, OH., and Metallurgical Society of AIME, Warrendale, PA.

Pub. in Fundamentals of Friction Wear of Materials, Pittsburgh, PA., October 4-5, 1981, Papers presented at the 1980 ASM Materials Science Seminar, p235-289.

Keywords: *Wear, Surface properties, Copper, Steels, Debris.

The paper describes the type of information that can be obtained from the characterization of worn specimens and the debris particles produced during wear. There are actually three potential sources for data and information - the worn surface, the subsurface volume, and the wear debris particles. The paper describes three different experiments carried out to develop an improved understanding of the wear of metals. In each case, the characterization methods applied were able to contribute necessary information to better understand the complete processes involved.

500,876

PB85-196038

Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

Quantitative Kinetic and Morphological Studies Using Model Systems.

Final rept.,

R. J. Schaefer, and M. E. Glicksman. 1981, 9p

Sponsored by Metallurgical Society of AIME, Warrendale, PA., and American Society for Metals, Metals Park, OH.

Pub. in Proceedings of a Symposium on Modeling of Casting and Welding Processes, Rindge, NH., August 3-8, 1980, p375-383 1981.

Keywords: *Solidification, Morphology, Dendritic crystals, Stability, Supercooling.

The usefulness for metallurgists of solidification studies using transparent model systems depends to a large extent on quantitative correlation to detailed theories of specific solidification phenomena. By designing experiments in which the thermal and geometrical conditions considered by the theory can be attained as closely as possible, and by making detailed kinetic and morphological measurements of the resulting solidification behavior, one can carry out incisive tests of the theory. Thus detailed study of dendritic growth in pure succinonitrile, together with auxiliary experiments which measured relevant thermodynamic properties, led to the important conclusion that the maximum velocity hypothesis for dendrite growth was not correct. This result has stimulated further theoretical work, which now appears to relate dendrite growth velocities to morphological stability considerations. Moreover, additional experimental and theoretical work is now revealing the regimes in which convection and solute effects are significant.

500,877

PB85-196251

Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

Calculations of Stable and Metastable Equilibrium Diagrams of the Ag-Cu and Cd-Zn Systems.

Final rept.,

J. L. Murray. 1984, 8p

Pub. in Metallurgical Transactions, A: Physical Metallurgy and Materials Science 15, n2 p261-268 Feb 84.

Keywords: *Silver alloys, *Copper alloys, *Cadmium alloys, *Zinc alloys, Phase diagrams, Equilibrium, Thermodynamics, Reprints.

Thermodynamic functions have been modeled for the binary alloy systems Ag-Cu and Cd-Zn, simple eutectic systems of interest in the areas of rapid solidification. Parameters of the thermodynamic functions are derived primarily from phase diagram data and compared to measured excess functions. Stable and metastable phase equilibria have been calculated, as well as the chemical spinodals and the locus of compositions and temperatures where liquid and solid have equal free energies.

500,878

PB85-197523

Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

EXAFS Study of the Passive Film on Iron.

Final rept.,

G. G. Long, J. Kruger, D. R. Black, and M. Kuriyama. 1983, 3p

Pub. in Jnl. of the Electrochemical Society 130, n1 p240-242 Jan 83.

Keywords: *Iron, *Corrosion, *Coatings, Solutions, Chromates, Nitrites, Crystalline structure, Vitreous state, Iron oxides, Reprints, *Extended X ray absorption fine structure.

A new surface EXAFS technique has been applied to the determination of the nature of the passive films formed on iron by chromate and nitrite passivating solutions. It found that the films formed that the EXAFS signatures of the passive films measured resemble those of the cubic spinel ferric oxides. The sharpness of the peaks, however, is significantly reduced from a crystalline structure, indicating that, at least the chromate-formed film is more vitreous than the model crystalline oxides.

500,879

PB85-197630

Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

Polymorphism of Nickel-Phosphorus Metallic Glasses.

Final rept.,

D. S. Lashmore, L. H. Bennett, H. E. Schone, P.

Gustafson, and R. E. Watson. 1982, 4p

Pub. in Physical Review Letters 48, n25 p1760-1763, 21 Jun 82.

Keywords: *Nickel alloys, Phosphoruscontaining alloys, Polymorphism, Frequency shift, Reprints, *Metallic glass, Amorphous materials.

It is shown that nickel-phosphorus metallic glass alloys not only exhibit two distinct local structural configurations for a given composition, but also that the configuration can be selected by choosing the appropriate processing parameters. It is also shown that the structure exhibiting the greater Knight shift exhibits a discontinuous transformation to the structure with the lower Knight shift. Measurements have been extended to alloys containing up to 42 atomic percent phosphorus.

500,880

PB85-202034

Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

Effect of Fluid Flow on Macroseggregation in Axi-Symmetric Ingots.

Final rept.,

S. D. Ridder, S. Kou, and R. Mehrabian. 1981, 13p

Pub. in Metallurgical Transactions B 12, n3 p435-447 Sep 81.

Keywords: *Ingots, *Continuous casting, Fluid flow, Mathematical models, Solidification, Separation, Heat transmission, Reprints.

A combined theoretical and experimental study of steady-state fluid flow, heat flow and segregation in axis-symmetric ingot production is presented, with specific applications in continuous casting and ESR. The fluid flow-segregation model involves the coupling of convective heat and fluid flow in the fully liquid metal pool ahead of the liquidus isotherm to the interdendritic fluid flow responsible for macrosegregation in the 'm ushy' zone of ingots solidifying under axis-symmetric conditions. Experiments on low-temperature Sn-Pb alloys verify the solidification model.

500,881

PB85-202059

Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

Diffusion-Induced Grain Boundary Migration in the Copper-Zinc System.

Final rept.,

T. J. Piccone, D. B. Butrymowicz, D. E. Newbury, J.

R. Manning, and J. W. Cahn. 1982, 5p

Pub. in Scripta Metallurgica 16, n7 p839-843 1982.

Keywords: *Copper alloys, *Diffusion, *Zinc, Grain boundaries, Microstructure, Metallography, Reprints.

Results are presented from an investigation of diffusion-induced grain boundary migration in the Cu-Zn system. Diffusion couples were prepared by annealing high-purity copper with brass powder. Zinc from the powder was diffused into the copper at temperatures at which grain boundary diffusion dominates and lattice diffusion is negligible. Boundary migration at or near the surface of the copper was examined through metallography, light microscopy, scanning electron microscopy, and the electron microprobe. Composition profiles across alloyed regions formed by boundary migration were determined with an electron microprobe and show unanticipated results.

500,882

PB85-203511

Not available NTIS

National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.

Relationships between Knoop and Scratch Micro-Indentation Hardness and Implications for Abrasive Wear.

Final rept.,

P. J. Blau. 1985, 21p

Pub. in Microstructural Science 12, p293-313 1985.

Keywords: *Microhardness tests, *Abrasion resistance, *Indentation hardness tests, *Wear, *Metals, Coatings, Loads(Forces), Correlations, Scratch hardness tests.

Micro-indentation hardness test methods are an important tool for the evaluation of thin metallic layers and coatings. Both vertically moving and horizontally moving (scratch) indentation methods are currently in wide use. An investigation was conducted on pure samples of Cu, Fe, Sn, Cd, Ni, and Co and on 1010 steel, 52100 steel, 638 bronze, 688 bronze, and Nitinol (NiTi alloy) to study the relationships between vertical and horizontal (scratch) micro-indentation hardness numbers. Indenter loads between 0.0098 and 0.196 N (10-200 g) were used. A standard Knoop indenter was

used for vertical testing and a 90 degree cone was used for scratch testing on a commercial scratch testing machine. Correlations between vertical and scratch hardness numbers varied with the testpiece material and the applied load. Microstructural features of the scratches were studied to analyze the cause of these variations. The implications of these variations for abrasive wear/microhardness number correlations are discussed.

500,883

PB85-205219

Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

Influence of a Multiple-Energy Ion Beam on the Equilibrium Profile of a Binary Alloy.

Final rept.,

M. L. Roush, F. Davarya, T. D. Andreadis, and O. F. Goktepe. 1983, 3p

Pub. in Jnl. of Vacuum Science and Technology A 1, n2 p491-493 1983.

Keywords: *Ion irradiation, Reprints, *Binary alloys, Ion bombardment.

Ion-bombardment-induced sputtering of a multi-element solid results in the preferential movement of the constituents, producing a composition profile which is dependent upon the beam energy. Recent studies have demonstrated transient changes in surface composition of such samples when the bombarding energy is abruptly changed. It is important to be able to treat multiple-energy ion beams since most sputtering systems have a contaminant of multiply-charged ions with higher energy than the principal component. The authors have studied the various competing processes that result in the equilibrium profile in order to develop the capability to predict the equilibrium profile which will result, once the parameters of the bombardment have been specified. They found that the equilibrium profile produced by a beam containing two energies cannot be obtained simply by interpolating between the two profiles that would result from the ion components individually. Interpolation is possible only in the near surface region.

500,884

PB85-205318

Not available NTIS

National Bureau of Standards, Gaithersburg, MD. Inorganic Materials Div.

Controlled Indentation Flaws for Construction of Toughness and Fatigue Master Maps.

Final rept.,

R. F. Cook, and B. R. Lawn. 1984, 21p

See also PB85-179042. Sponsored by Office of Naval Research, Arlington, VA.

Pub. in American Society for Testing and Materials, Special Technical Publication 844, p22-42 1984.

Keywords: *Toughness, *Fatigue(Life), *Life(Durability), *Defects, Indentation, Crack propagation, Predictions, Graphs(Charts), Failure, Stresses.

A simple and economical procedure for accurate determinations of toughness and lifetime parameters is described. Indentation flaws are introduced into strength test pieces, which are then taken to failure under specified stressing and environmental conditions. By controlling the size of the critical flaw, via the contact load, material characteristics can be represented universally on 'master maps' without the need for statistical considerations. The paper surveys both the theoretical background and the experimental methodology associated with the scheme. The theory is developed for 'point' flaws for dynamic and static fatigue, incorporating load explicitly into the analysis. A vital element of the fracture mechanics is the role played by residual contact stresses in driving the cracks to failure. Experimental data on a range of Vickers-indented glasses and ceramics are included to illustrate the power of the method as a means of graphic materials evaluation. It is demonstrated that basic fracture mechanics parameters can be measured directly from the slopes, intercepts and plateaus on the master maps, and that these parameters are consistent, within experimental error, with macroscopic crack growth laws.

500,885

PB85-207108

Not available NTIS

National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.

Novel Double-Peaked Spin-Glass Susceptibility - Temperature Response in the Ternary Alloy Fe₆₉Mn₂₆Cr₅.

Final rept.,

T. Datta, D. Thornberry, E. R. Jones, and H. M.

Ledbetter. 1984, 3p

Contract NSF-ISP80-11451

Sponsored by South Carolina Univ., Columbia, National Aeronautics and Space Administration, Washington, DC. and Department of Energy, Washington, DC. Office of Fusion Energy.

Pub. in Solid State Communications 52, n5 p515-517 1984.

Keywords: *Austenitic stainless steels, Magnetic permeability, Phase transformations, Reprints.

The authors have studied the low-field ($B < \text{or} = 10$ to the minus 2 power T) d.c. susceptibility χ of the austenitic stainless-steel alloy Fe₆₉Mn₂₆Cr₅ as a function of the magnetic field B and temperature T. $\chi(T)$ shows structure, strong B dependence, and typical irreversible effects. The range of temperatures studied comprises three distinct regions.

500,886

PB85-207132

Not available NTIS

National Bureau of Standards (NEL), Gaithersburg, MD. Thermophysics Div.

Thermal Expansion of Iron during the alpha yields gamma Phase Transformation by a Transient Interferometric Technique.

Final rept.,

A. P. Müller, and A. Cezairliyan. 1984, 14p

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

Pub. in Thermal Expansion 8, p245-258 1984.

Keywords: *Iron, *Thermal expansion, Phase transformations, Measurement, Reprints.

Measurements of thermal expansion of iron in the vicinity of (and during) the alpha to gamma phase transformation have been performed by a transient (subsecond) interferometric technique. The basic method involves rapidly heating the specimen from room temperature up to about 1300 K in less than one second by the passage of an electrical current pulse through it, and simultaneously measuring the specimen expansion by the shift in the fringe pattern produced by a Michelson-type interferometer and the specimen temperature by means of a high-speed photoelectric pyrometer.

500,887

PB85-207181

Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

Sub-Surface Hardening in Erosion-Damaged Copper As Inferred from the Dislocation Cell Structure, and Its Dependence on Particle Velocity and Angle of Impact.

Final rept.,

D. Kuhlmann-Wilsdorf, and L. K. Ives. 1983, 13p

Pub. in Wear 85, n3 p361-373 1983.

Keywords: *Copper, Hardening(Materials), Erosion, Dislocations(Materials).

Previously published measurements of the cell diameters (d) of dislocation cells underneath copper surfaces exposed to particle erosion have been evaluated in terms of the subsurface stresses to which they correspond. These were compared with the elastic stresses expected underneath spherical indentors impacting on the surface with different speeds. The inferred stresses differ markedly from theoretical prediction, not only in regard to dependence on speed and angle of impact, but even in regard to their decay along the z-axis, the direction normal to the surface.

500,888

PB85-207967

Not available NTIS

National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.

Anomalous Low-Temperature Elastic-Constant Behaviour of Fe-20Cr-16Ni-6Mn.

Final rept.,

H. M. Ledbetter, and M. W. Austin. Nov 84, 4p

See also PB80-178403. Sponsored by Department of Energy, Washington, DC. Office of Fusion Energy and National Science Foundation, Washington, DC.

Pub. in Metal Science 18, p539-542 Nov 84.

Keywords: *Austenitic stainless steels, Elastic properties, Bulk modulus, Cryogenics, Low temperature research, Phase transformations, Neel temperature,

Shear modulus, Poisson ratio, Reprints, Steel 20Cr 6Mn 16Ni.

For the high nickel content austenitic stainless steel Fe-20Cr-16Ni-6Mn (wt-%), the complete set of polycrystalline elastic constants between 295 and 4 K were determined ultrasonically. A reversible magnetic transition occurs near 54 K. During cooling, the bulk modulus begins to soften at a much higher temperature, near 150 K. Local moments above the transition temperature may explain this peculiarity.

500,889

PB85-207975

Not available NTIS

National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.

Predicted Monocrystal Elastic Constants of 304-Type Stainless Steel.

Final rept.,

H. M. Ledbetter. 1985, 4p

Sponsored by Department of Energy, Washington, DC. Office of Fusion Energy.

Pub. in Physica 128B, p1-4 1985.

Keywords: *Stainless steels, Elastic properties, Kroner method, Steel 304.

The three monocrystal elastic constants C_{11} , C_{12} , C_{44} of 304-type stainless steel are estimated from the polycrystalline bulk and shear moduli together with an empirical C_{12}/C_{11} value, which is discussed theoretically. The estimate involves a reverse Kroner method for relating monocrystal and polycrystal elastic constants.

500,890

PB85-207983

Not available NTIS

National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.

Monocrystal-Polycrystal Elastic Constants of a Stainless Steel.

Final rept.,

H. M. Ledbetter. 1984, 8p

Sponsored by Department of Energy, Washington, DC. Office of Fusion Energy.

Pub. in Physica Status Solidi (a) 85, p89-96 1984.

Keywords: *Nickel chromium steels, *Stainless steels, Elastic properties, Reprints, Steel 19Cr 10Ni.

For a face-centered-cubic steel, new measurements of the monocrystal Voigt elastic-stiffness constants C_{11} , C_{12} , C_{44} are given. The monocrystal steel, Fe-19Cr-10Ni, corresponds closely to the well-known AISI-304 austenitic stainless steel. Considering seven theories for the monocrystal-polycrystal elastic constants, it is found that the Hershey-Kroner-Eshelby theory agrees best with measurements. It predicts the shear modulus within 2% of observation, where the Voigt-Reuss first-order bounds differ by 49%. Ten sets of Fe-Cr-Ni C_{ij} results are reviewed with the finding that both Zener's elastic anisotropy and the C_{12}/C_{11} ratio are constant within 5%.

500,891

PB85-227650

Not available NTIS

National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.

Microanalytical Study of Secondary Precipitation in RSR 143 Using Atom Probe Field Ion Microscopy and Analytical Transmission Electron Microscopy.

Final rept.,

M. E. Twigg, A. J. Melmed, R. Klein, M. J. Kaufman,

and H. L. Fraser. 1984, 6p

Pub. in Proceedings of Int. Symp. Superalloys (5th), Champion, PA., October 7-11, 1984, p631-636 1984.

Keywords: *Precipitation(Chemistry), *Heat resistant alloys, *Heat treatment, *Chemical analysis, Nickel alloys, Phase transformations, Chemical composition, Stabilization, Tantalum, Aluminum, Solid solutions, Solids, Microanalysis, *Nickel alloy RSR 143, *Superalloys, Atom probe field ion microscopy, Transmission electron microscopy, Long range interactions.

For a given heat treatment, the Ni-base superalloy RSR 143 consists of three phases: the gamma matrix, gamma prime cuboids, and DO(22) platelets. Atom probe field ion microscopy and analytical transmission electron microscopy are used in determining the compositions of these three phases.

500,892

PB85-229375

Not available NTIS

Field 11—MATERIALS

Group 11F—Metallurgy and Metallography

National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.

Convective Influence on the Stability of a Cylindrical Solid-Liquid Interface.

Final rept.,
Q. T. Fang, M. E. Glicksman, S. R. Coriell, G. B. McFadden, and R. F. Boisvert. 1985, 21p
Sponsored by National Aeronautics and Space Administration, Washington, DC.
Pub. in Jnl. of Fluid Mechanics 151, p121-140 1985.

Keywords: *Interfaces, Solids, Liquid metals, Fluid flow, Convection, Grashof number, Stability, Melts, Crystal growth, Reprints, Instability.

Experiments in which a long vertical, heated wire is surrounded by concentric annuli of a melt and its crystalline solid show that the convection state changes from a stable unicell surrounded by a stationary cylindrical solid-liquid interface, to a complex time-dependent flow surrounded by a rotating, helical solid-liquid interface. A linear stability analysis has been carried out for an infinitely tall vertical annulus. When the deformable nature of the crystal-melt interface is taken into account in the boundary conditions, two new modes of instability arise.

500,893

PB85-229425 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.

Effect of a Forced Couette Flow on Coupled Convective and Morphological Instabilities during Unidirectional Solidification.

Final rept.,
S. R. Coriell, G. B. McFadden, R. F. Boisvert, and R. F. Sekerka. 1984, 9p
Sponsored by National Aeronautics and Space Administration, Washington, DC.
Pub. in Jnl. of Crystal Growth 69, n1 p15-22 Nov 84.

Keywords: *Solidification, *Lead alloys, Couette flow, Tin containing alloys, Convection, Interfaces, Melts, Crystal growth, Reprints, Instability.

The effect of a forced Couette flow, parallel to a horizontal crystal-melt interface during directional solidification of an alloy of lead containing tin, on the onset of convective and morphological instabilities, is calculated numerically via a linear stability analysis. Such a flow does not affect perturbations with wave vectors perpendicular to the flow. For perturbations with wave vectors parallel to the flow, the onset of morphological instability is somewhat suppressed and thermosolutal convection is greatly suppressed. When instabilities occur, they are oscillatory and correspond to travelling waves. For values of the crystal growth velocity for which mixed morphological and convective modes occur, the presence of a forced flow produces sufficient decoupling to allow otherwise degenerate branches to be identified.

500,894

PB85-229995 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Thermophysics Div.

Thermophysical Measurements on Tungsten-3 (Wt %) Rhenium Alloy in the Range 1500-3600 K by a Pulse Heating Technique.

Final rept.,
A. Cezairliyan, and A. P. Müller. 1985, 13p
Sponsored by Air Force Office of Scientific Research, Bolling AFB, DC.
Pub. in International Jnl. of Thermophysics 6, n2 p191-202, 27 Sep 85.

Keywords: *Tungsten alloys, Rhenium containing alloys, Specific heat, Electrical resistivity, Emittance, Thermal measurement, Reprints, Tungsten alloy 3Rh.

Simultaneous measurements of the specific heat capacity, electrical resistivity, and hemispherical total emittance of tungsten-3 (wt%) rhenium alloy in the temperature range 1500-3600K by a subsecond-duration pulse heating technique are described.

500,895

PB85-230647 Not available NTIS
National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.

Effects of Carbon and Nitrogen on the Elastic Constants of AISI (American Iron and Steel Institute) Type 304 Stainless Steel.

Final rept.,
H. M. Ledbetter, and M. W. Austin. 1985, 8p
Sponsored by Department of Energy, Washington, DC. Office of Fusion Energy.

Pub. in Materials Science and Engineering 70, p143-149 1985.

Keywords: *Stainless steels, Elastic properties, Carbon, Nitrogen, Reprints, Steel 304.

Nine AISI type 304 stainless steel alloys were studied at room temperature. The carbon-plus-nitrogen contents of these alloys ranged from 0.067 to 0.325 wt.% (from 0.3 to 1.3 at. %). Five elastic constants (the longitudinal modulus, Young's modulus, the shear modulus, the bulk modulus and Poisson's ratio) were determined by a pulse echo ultrasonic method.

500,896

PB86-102399 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.

Cellular Growth During Directional Solidification.

Final rept.,
S. R. Coriell, G. B. McFadden, and R. F. Sekerka. 1985, 27p
Grant NSF-DMR84-09397
Sponsored by Defense Advanced Research Projects Agency, Arlington, VA.
Pub. in Annual Review of Materials Science 15, p119-145 1985.

Keywords: *Solidification, *Crystal growth, Binary systems(Materials), Alloys, Stability, Reprints.

During directional solidification of an alloy, a planar crystal-melt interface may become unstable and develop into a cellular or dendritic interface; the resulting crystal is then non-uniform in solute concentration with spatial inhomogeneities transverse to the growth direction. Linear morphological stability predicts the conditions and the wavelength at the onset of instability. The linear theory and recent extensions of it are reviewed. Recent theoretical advances in the non-linear aspects of the free boundary problem associated with directional solidification are discussed. Recent experimental tests of the linear theory and measurements of cellular wavelengths in binary alloys are described.

500,897

PB86-111010 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.

Basic Aspects of the Problems of Hydrogen in Steels.

Final rept.,
C. G. Interrante. 1982, 15p
Pub. in Proceedings of International Conference on Current Solutions to Hydrogen Problems in Steels (1st), Washington, DC., November 1-5, 1982, p3-17.

Keywords: *Hydrogen embrittlement, *Steels, *Blistering, Diffusion, Transport properties, Surface chemistry, Solubility, Absorption.

The solubility, diffusion, and permeation of hydrogen in steels, the various proposed mechanisms of hydrogen embrittlement and attack, some of the prominent observed effects of hydrogen on the properties and behavior of steels, and some understanding of the ways in which hydrogen interacts with steels are described herein. Basic aspects of the problem involve the limited solubility of hydrogen, the adsorption of hydrogen on both internal and external steel surfaces, the absorption into the steel lattice, the transport of hydrogen by diffusion and by the motion of dislocations, and the localization of hydrogen at internal sites in the bulk metal. This localization may be as adsorbed hydrogen atoms on surfaces, as molecular hydrogen that exerts a gas pressure in void spaces, or as interstitial hydrogen in solution. While our overall understanding of the mechanisms that explain the harmful effects is incomplete, the proposed mechanisms furnish a context within which we can view the problem and classify the observed behavior and effects of hydrogen in steels.

500,898

PB86-111994 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.

Analysis of Interlaboratory Test Results of Solid Particle Impingement Erosion.

Final rept.,
A. W. Ruff. 1985, 7p
Pub. in Wear of Materials 1985, p654-660 1985.

Keywords: *Erosion, Impingement corrosion, Tests, Steels, Measurements, Test equipment, Particles.

During the development of a standard method for solid particle impingement erosion testing of materials, a

number of interlaboratory test comparisons were conducted. The paper describes the results of four test series involving twelve laboratories in total. The measurements were carried out with considerable care using the gas jet type of erosion tester, involving nearly the same conditions and test parameters on two different materials, a low carbon steel and a stainless steel.

500,899

PB86-112869 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.

Environmental Testing under Conditions That Promote Crack Branch Formation in Side-Grooved, Double-Beam Specimens.

Final rept.,
C. G. Interrante, and S. R. Low. 1982, 6p
Pub. in Hydrogene Mater., 3rd Int. Congr. 2, p557-562 1982.

Keywords: *Cracking(Fracturing), *Steels, Environmental tests, Crack propagation, Hardness, Inclusions, Hydrogen embrittlement.

Side-grooved, double-beam specimens of a 2 1/4 Cr - 1 Mo steel were tested under severe charging conditions that promoted the formation of branch cracks in test specimens of four orientations, which are designated S-T, S-L, T-L, and L-T. These branch cracks depart from the intended plane of cracking as they propagate into one of the beams of the specimen, and when this condition is severe it can preclude the development of meaningful data. The general tendency for branch crack formation was observed to increase with increasing hardness of the test specimen.

500,900

PB86-112877 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.

Hydrogen Absorption by 2 1/4Cr-Mo Steel in Acidified H₂S Environments.

Final rept.,
J. A. Kargol, and C. G. Interrante. 1982, 9p
Pub. in Proceedings of International Conference (1st) on Current Solutions to Hydrogen Problems in Steels, Washington, DC., November 1-5, 1982, p438-446.

Keywords: *Steels, Hydrogen, Absorption, Cracking(Fracturing), Permeating, Hydrogen embrittlement, Hydrogen sulfide.

No abstract available.

500,901

PB86-113602 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.

Basic Mechanisms of Atomic Redistribution in Alloys Undergoing Irradiation.

Final rept.,
J. R. Manning. 1981, 19p
Pub. in Proceedings of Phase Stability During Irradiation, Pittsburgh, PA., October 5-9, 1980, p3-21 1981.

Keywords: *Point defects, *Crystal defects, *Diffusion theory, *Irradiation, *Segregation process, Alloys, *Physical radiation effects.

In alloys undergoing irradiation, vacancies and interstitials can be created in great numbers by radiation damage processes. These point defects then migrate and produce large defect fluxes directed from the interior of the alloy to grain boundaries, pores and the alloy surface. The resulting vacancy and interstitial fluxes can appreciably affect diffusion processes and cause significant solute redistribution, even in originally homogeneous alloys. In this paper, basic driving forces and diffusion equations governing this process are discussed. Two distinct forces which arise from the irradiation-produced defects can be identified: (1) steady state macroscopic defect concentration gradients affect the basic atom jump frequencies, and (2) defect fluxes, especially if the fluxes are non-uniform in character, change the local microscopic defect distributions around individual atoms and alter the effective atom jump frequencies. A general equation for the steady state segregation gradient in binary alloys is presented, and simple applications are made to dilute alloys.

500,902

PB86-119328 Not available NTIS
National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.

Fatigue Crack Growth of a Ship Steel in Seawater under Spectrum Loading.

Final rept.,
Y. W. Cheng. 1985, 6p
Sponsored by Minerals Management Service, Reston, VA.
Pub. in International Jnl. of Fatigue 7, n2 p95-100 1985.

Keywords: *Structural steels, *Fatigue(Materials), *Crack propagation, *Sea water corrosion, *Environmental tests, *Ship structural components, Offshore structures, Loads(Forces), North Sea, Mechanical properties, Reprints.

Fatigue crack growth of ABS EH36 steel under spectrum loading intended to simulate sea loading of offshore structures in the North Sea was studied using fracture mechanics. A digital simulation technique was used to generate samples of load/time histories from a power spectrum characteristic of the North Sea environment. The procedure is equivalent to applying Miner's summation rule in fatigue life calculations.

500,903

PB86-123056

Not available NTIS

National Bureau of Standards (NML), Gaithersburg, MD. Temperature and Pressure Measurements and Standards Div.

Coin Silver as a Construction Material in Low-Temperature Experiments.

Final rept.,
C. T. Van Degrieff. 1981, 2p
Pub. in Proceedings of International Conference on Low Temperature Physics LT-16 (16th), Los Angeles, CA., August 19-25, 1981, Physica B+C 107, n1-3 p605-606 Aug/Sep 81.

Keywords: *Coin silver, Construction materials, Low temperature tests, Physical properties.

The utility of an alloy of 10% copper in silver (coin silver) as a construction material in certain low temperature experiments is discussed. While maintaining low-temperature thermal and electrical conductivities between copper and brass, this easily machined alloy has very little magneto-resistance, 10% of the magnetic specific heat of copper, and is highly resistant to creeping under mechanical stress. A table of the low-temperature properties of coin silver is presented which includes the results of direct measurements of its magneto-thermal conductivity below 500 mK.

500,904

PB86-124138

Not available NTIS

National Bureau of Standards (NML), Gaithersburg, MD. Inorganic Analytical Research Div.

Isotope Dilution Spark Source Mass Spectrometric Determination of Sulfur in Selected NBS (National Bureau of Standards) Iron-Base Alloys.

Final rept.,
P. J. Paulsen, R. W. Burke, E. J. Maienthal, and G. M. Lambert. 1981, 8p
Sponsored by American Society for Testing and Materials, Philadelphia, PA.
Pub. in American Society for Testing and Materials, Special Technical Publication 747, p113-120 1981.

Keywords: *Chemical analysis, *Isotopic labeling, *Sulfur, *Iron containing alloys, Sampling, Mass spectroscopy, Chemical equilibrium, Physical properties, Hydrogen sulfide, Silver sulfides, Metals, Concentration(Composition), Reprints, *Isotope dilution spark source mass spectroscopy.

A procedure has been developed at NBS utilizing spark source mass spectrometric (SSMS) isotope dilution for the determination of sulfur in iron-base alloys. With this technique a known amount of highly enriched (Sup 34)S isotope (spike) is added to the sample and, following physical and chemical equilibration between the spike sulfur and the natural sulfur in the sample, the equilibrated sulfur is isolated by reduction to H₂S and precipitation as Ag₂S. The altered isotopic ratio of the sulfur (Sup 34)S/(Sup 32)S is then measured with the SSMS. Sulfur concentrations are calculated from the sample weight, spike weight, measured altered isotope ratio, and known isotopic abundance of (Sup 34)S and (Sup 32)S in both natural and spike sulfur. The key step in obtaining a quantitative sulfur analysis is the dissolution of the sulfur-containing iron samples in a sealed tube. This dissolution procedure enables the sample sulfur and the spike sulfur to completely equilibrate without any possibility of loss of either species by volatilization.

500,905

PB86-124146

Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

National Cost of Automobile Corrosion.

Final rept.,
E. Passaglia, and R. A. Haines. 1980, 13p
Sponsored by National Association of Corrosion Engineers, Houston, TX.
Pub. in Proceedings of Corrosion/80 International Corrosion Forum Devoted Exclusively to the Protection and Performance of Materials, Chicago, IL., March 3-7, 1980, p118.1-118.13.

Keywords: *Automobiles, *Corrosion, Expenses, *Costs, Maintenance costs.

The costs of automobile corrosion presented in the NBS report, 'Economic Effects of Metallic Corrosion in the United States' have been collected from that report and presented separately. Costs are given as incurred by the automobile manufacturing sector for corrosion resistant inputs such as copper and stainless steel, and as incurred by the industrial sectors, the private consumer, the Federal Government and state and local government for maintenance and shortened lifetime. Total costs are given as well as the portion that is avoidable by the use of economic best practice. The uncertainties in the estimates of the costs and their origins are discussed.

500,906

PB86-124161

Not available NTIS

National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.

Beryllium Microdeformation Mechanisms.

Final rept.,
R. S. Polvani, B. W. Christ, and E. R. Fuller. 1981, 11p
See also AD-A111 499. Sponsored by Office of Naval Research, Boston, MA.
Pub. in Proceedings of International Conference on Creep and Fracture of Engineering Materials and Structures, Swansea, Wales, March 24-27, 1981, p85-95.

Keywords: *Beryllium, *Deformation, Dimensional measurement, Tensile strength, Creep properties.

Microtensile and microcreep behaviors of beryllium were studied using a capacitance type extensometer capable of resolving .1 um/m over long times. The nature of the dislocation processes responsible for microdeformation are not entirely clear; but surely, the primary difference between micro and conventional deformation is the extent to which the dislocations move and not the nature of the processes. Despite low temperatures, microcreep of Instrument Grade Beryllium appears to be diffusion limited.

500,907

PB86-124963

Not available NTIS

National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.

Processing/Microstructure Relationships in Surface Melting.

Final rept.,
R. J. Schaefer, and R. Mehrabian. 1983, 12p
Pub. in Proceedings of Laser-Solid Interactions and Transient Thermal Processing of Materials, Boston, MA., November 1-4, 1982, v13 p733-744 1983.

Keywords: Melting, Electron beam melting, Homogeneity, Aluminum, Interfaces, Stability, Solidification, Microstructure, Process control, *Surface melting, Rapid solidification.

The development of predictive models for rapid surface melting and resolidification requires coupling of realistic heat flow models to emerging theories of rapid solidification processing. An overview is given of the emerging guidelines for prediction and control of rapid solidification conditions and microstructures. Homogenization of the liquid by convection and diffusion is also discussed. Electron beam surface melting of alloy substrates is used as an example of these processes.

500,908

PB86-128196

Not available NTIS

National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.

Fatigue Crack Growth of Duplex Stainless Steel Castings at 4 K.

Final rept.,
P. T. Purtscher, Y. W. Cheng, and P. N. Li. 1985, 5p
Sponsored by Department of Energy, Washington, DC. Office of Fusion Energy.

Pub. in Jnl. of Engineering Materials and Technology 107, p161-165 Apr 85.

Keywords: *Stainless steels, *Crack propagation, Cryogenics, Fatigue(Materials), Reprints.

Constant-load-amplitude stage II fatigue crack growth rates at 4 K were measured for duplex stainless steel castings. The results show that at a delta K of 60 MPa(m to the 1/2 power), da/dN = 0.00076 mm/cycle for an alloy with 1 percent ferrite. For an alloy with 8 percent ferrite, da/dN is 35 percent, and for an alloy with 29 percent ferrite, da/dN is 260 percent greater than for the 1 percent ferrite alloy.

500,909

PB86-128253

Not available NTIS

National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.

Rapid Solidification.

Final rept.,
R. Mehrabian. 1982, 24p
International Metals Reviews 27, n4 p185-208 1982.

Keywords: Solidification, Phase diagrams, Process control, Powder metallurgy, Nondestructive tests, Microstructure, Heat transmission, *Rapid solidification.

Points of progress in current understanding of rapid liquid to solid transformation are reviewed. Emphasis is placed on those aspects of the emerging science that would permit development of guidelines and predictive models for alloy design and process control to achieve desired microstructures and properties.

500,910

PB86-128881

Not available NTIS

National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.

Comment on 'The Elastic Stiffness Coefficients of Nickel-Iron Single-Crystal Alloys at Room Temperature'.

Final rept.,
H. M. Ledbetter. 1985, 2p
Sponsored by Department of Energy, Washington, DC. Office of Fusion Energy.
Pub. in Jnl. of Applied Physics 57, n11 p5069-5070, 1 Jun 85.

Keywords: *Iron alloys, *Nickel alloys, *Shear properties, Face centered cubic lattices, Elastic properties, Single crystals, Poisson ratio, Phase transformations, Magnetic properties, Reprints.

The author responds to the recent claim that in face-centered-cubic Fe-Ni alloys the two cubic elastic-shear coefficients, C₄₄ and (C₁₁-C₁₂)/2, vary linearly with composition. Both theory and measurement support a nonlinear variation.

500,911

PB86-128899

Not available NTIS

National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.

Manganese Contributions to the Elastic Constants of Face Centred Cubic Fe-Cr-Ni Stainless Steel.

Final rept.,
H. M. Ledbetter. 1985, 7p
Sponsored by Department of Energy, Washington, DC. Office of Fusion Energy.
Pub. in Jnl. of Materials Science 20, p2923-2929 1985.

Keywords: *Stainless steels, *Elastic properties, *Manganese containing alloys, Mechanical properties, Poisson ratio, Ultrasonic tests, Bulk modulus, Reprints.

The author determined experimentally the effect of manganese on the elastic constants of face centred cubic Fe-Cr-Ni alloys with chemical compositions near 304-type stainless steel. By a pulse-echo-overlap method, longitudinal and transverse soundwave velocities were determined in ten alloys containing up to 6% manganese. All the elastic stiffnesses decrease linearly with increasing manganese. The bulk modulus decreases most strongly. Poisson's ratio changes least. We consider what the elastic constants reveal concerning changes in chemical bonding, caused by manganese additions.

500,912

PB86-128907

Not available NTIS

National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.

Field 11—MATERIALS

Group 11F—Metallurgy and Metallography

Elastic Constant Versus Temperature Behavior of Three Hardened Maraging Steels.

Final rept.,
H. M. Ledbetter, and M. W. Austin. 1985, 5p
Sponsored by National Aeronautics and Space Administration, Langley Station, VA. Langley Research Center, and Department of Energy, Washington, DC. Office of Fusion Energy.
Pub. in Materials Science and Engineering 72, p65-69 1985.

Keywords: *Elastic properties, *Maraging steels, Bulk modulus, Shear modulus, Poisson ratio, Reprints, *Temperature effects, Ultrasonic velocity.

Elastic constants of three maraging steels were determined by measuring ultrasonic velocities. Annealed steels show slightly lower bulk moduli and considerably lower shear moduli than hardened steels.

500,913
PB86-129558 PC A03/MF A01
General Electric Co., Schenectady, NY. Materials Information Services.
Standards and Metadata Requirements for Computerization of Selected Mechanical Properties of Metallic Materials.

Final rept.,
J. H. Westbrook. Aug 85, 50p NBS/SP-702
Library of Congress catalog card no. 85-600585. Also available from Supt. of Docs as SN003-003-02691-3. Sponsored by National Bureau of Standards (NML), Gaithersburg, MD. Office of Standard Reference Data, and Army Materiel Development and Readiness Command, Alexandria, VA.

Keywords: *Standards, *Metals, Mechanical properties, Tests, Computer applications.

To assist in building a computerized information system on the engineering properties of materials, the standards and metadata requirements for a representative group of mechanical property categories are considered. These categories include: tensile behavior, hardness numbers, notch-bar impact test parameters and fatigue properties. For each property group, definitions of terms, synonyms (and non-synonyms), standard test methods, standards for reporting data, precision and accuracy, and correlations of properties are addressed. The principal findings and recommendations are as follows. Existing test methods are generally adequate for the properties considered but better standards are needed for data reporting. Appraisal of materials variability and testing machine variability would be assisted by access to standard reference materials, certified as to their mechanical properties.

500,914
PB86-130101 Not available NTIS
National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.
Numerical and Experimental Verification of Compliance Functions for Compact Specimens.
Final rept.,
R. L. Tobler, and W. C. Carpenter. 1985, 10p
Sponsored by Department of Energy, Washington, DC. Office of Fusion Energy.
Pub. in Engineering Fracture Mechanics 21, n3 p547-556 1985.

Keywords: *Modulus of elasticity, Numerical analysis, Mechanical properties, Cracking(Fracturing), Reprints, Finite element analysis.

A two-dimensional finite element study of the compact specimen was performed in verification of its elastic compliance calibration functions. The results confirm Newman's boundary collocation solutions to within 2%. Empirical calibrations were also performed using alloys with well-known elastic moduli. The numerical and empirical agreement depends on the state of stress assumed in the model, with better agreement for plane stress than for plane strain.

500,915
PB86-130119 Not available NTIS
National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.
Interstitial Carbon and Nitrogen Effects on the Cryogenic Fatigue Crack Growth of AISI 304 Type Stainless Steels.
Final rept.,
R. L. Tobler, and R. P. Reed. 1984, 7p
Pub. in Jnl. of Testing and Evaluation 12, n6 p364-370 Nov 84.

Keywords: *Crack propagation, *Stainless steels, Low temperature tests, Cryogenics, Carbon, Nitrogen, Me-

chanical properties, Fatigue(Materials), Reprints, Steel 304.

Constant-load-amplitude fatigue crack propagation (FCP) rate measurements are reported for AISI 304 (Unified Numbering System (UNS) S30400) type stainless steels having variable carbon-plus-nitrogen (C+N) contents. The improved cryogenic behavior at low C+N contents was associated with a transition in failure micromechanisms.

500,916
PB86-132594 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.
Modeling of Crack Chemistry in the Alpha Brass-Ammonia System.

Final rept.,
U. Bertocci. 1984, 10p
Pub. in Proceedings of International Symposium Fall Meeting of Metallurgy Society, Embrittlement Localized Crack Environment, p49-58 1984.

Keywords: *Stress corrosion, Brass, Ammonia, Hydrogen, Electric potential, Concentration(Composition).

Concentration and electrical potential profiles generated in a crack by anodic dissolution of alpha-brass in aqueous ammonia have been calculated for stationary conditions, taking into account both diffusion and electromigration. Hydrogen discharge following instantaneous crack advance, which exposes fresh brass surface to the solution, has also been considered. From the equivalent circuit, the values at the crack-tip have been obtained for a range of kinetic parameters and surface area ratios.

500,917
PB86-132651 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.
Competition between Wear Processes during the Dry Sliding of Two Copper Alloys on 52100 Steel.
Final rept.,
P. J. Blau. 1983, 8p
Pub. in Proceedings of Wear of Materials Conference, Reston, VA., April 11-14, 1983, p526-533.

Keywords: *Wear, *Copper alloys, Steels, Sliding, Tests, Friction, Microhardness.

More than one wear process may be operating simultaneously during the dry sliding of metals. Moreover, the relative contributions of these processes may change with time. Flat blocks of two commercial alloys of copper (CDA 638 and 688) were held against rotating rings of 52100 steel under a normal load of 10 N and 20 cm/s velocity for a series of tests in Ar gas environments. Microscopy revealed two different operating wear processes on the alloy 638 wear scars. Separate wear volumes were computed for the two mechanisms (metallic and dull-colored wear zones). Microhardness gradients were obtained below these zones.

500,918
PB86-133543 Not available NTIS
National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.

Properties and Performance of Candidate Structural Metals for the Production of Synthetic Gas from Coal.

Final rept.,
B. W. Christ, H. Ondik, A. Perloff, and B. Beck. 1983, 15p
Sponsored by Department of Energy, Washington, DC. Office of Fossil Energy, and Department of Energy, Laramie, WY. Laramie Energy Technology Center.
Pub. in Proceedings of 1983 International Gas Research Conference, London, England, June 13-16, 1983, p456-470.

Keywords: *Coal gasification, *Construction materials, *Corrosion environment, *Materials tests, Structural analysis, Mechanical properties, Design criteria, Sites, Performance evaluation.

Data from several nationwide (U.S.) Department-of-Energy-sponsored programs have been collected and evaluated by the DoE-sponsored Materials Performance Center at the U.S. National Bureau of Standards. New and traditional alloys, about 60 of them, were evaluated. Laboratory measurements and in-plant measurements were made of the following properties: hot gas corrosion rates, aqueous corrosion rates, erosion-corrosion rates, aqueous corrosion rates, and me-

chanical properties in a coal gasification environment. Highlights of these data will be discussed in light of design needs at critical plant locations. Furthermore, test methodologies and opportunities for standardization will be discussed.

500,919
PB86-138096 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Mathematical Analysis Div.
Computer Software Needs of Materials Property Data Bases for Selected Engineering Applications.
Final rept.,
J. T. Fong. 1983, 31p
Pub. in Proceedings of Winter Annual Meeting of the American Society of Mechanical Engineers - On-Line Materials Property Data Base, Boston, MA., November 13-18, 1983, p75-105.

Keywords: *Engineering, *Computer graphics, *Materials, Properties, Economics, Stainless steels, Metal products, *Computer software, *Data bases, File management systems, User needs.

The technical opportunities and economic constraints in the development of materials property data bases and networks for engineering applications are examined. Factors that are likely to influence a typical engineer-user to supplement or supplant handbooks with data bases are discussed to support a proposition that engineering-oriented information systems need sophisticated softwares to ensure (a) credibility, (b) flexibility, and (c) faithful representation of the 'hard' and 'soft' texture of the data.

500,920
PB86-140035 Not available NTIS
National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.
Midrange Fatigue Crack Growth Data Correlations for Structural Alloys at Room and Cryogenic Temperatures.
Final rept.,
R. L. Tobler, and Y. W. Cheng. 1985, 26p
Sponsored by Department of Energy, Washington, DC. Office of Fusion Energy.
Pub. in Fatigue at Low Temperatures, ASTM STP 857, p5-30 1985.

Keywords: *Structural steels, *Crack propagation, Cracking(Fracturing), Fatigue(Materials), Austenitic stainless steels, Cryogenics, Modulus of elasticity, Reprints.

Fatigue crack growth rate data for pure metals, structural alloys, and welds at temperatures from 295 to 4K are selectively reviewed. The data for more than 200 material and temperature combinations are discussed in terms of the parameters C and n for the midrange of the da/dN-versus-Delta K curve. Fatigue resistance varies greatly among the different alloy classes and crystal structure types, especially at extreme cryogenic temperatures, where alternative failure mechanisms emerge. Good general correlations were achieved on the basis of Young's modulus, fracture toughness, and empirical equations relating C and n for each alloy class.

500,921
PB86-140316 Not available NTIS
National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.
Fracture Toughness and Microstructure of a Martensitic High Carbon Alloy Steel.
Final rept.,
P. T. Purtscher, and G. Krauss. 1985, 16p
Sponsored by Bethlehem Steel Corp., PA.
Pub. in Proceedings of the Symposium on Fracture: Interactions of Microstructure, Mechanisms and Mechanics, Los Angeles, California, February 27-29, 1984, p179-194 1985.

Keywords: *Carbon steels, Fracture properties, Microstructure, High strength steels, Austenitizing, Steel AISI 4485.

The toughness of AISI 4485 steel was evaluated as a function of austenitizing temperature between 800 and 950C. Increasing austenitizing temperature coarsened and reduced the volume fraction of spherical carbides retained after hardening. The shape of the curves is discussed relative to the changes in microstructure and fracture morphologies observed. An analysis technique based upon the energy required for crack growth is applied that describes the defect tolerance of the

steel more completely than the ASTM E399 procedure.

500,922

PB86-142882

Not available NTIS

National Bureau of Standards (NEL), Gaithersburg, MD. Building Materials Div.

Nondestructive Evaluations of Steel Corrosion under Protective Coatings Using Thermal-Wave Imaging.

Final rept.,

T. Nguyen. 1985, 10p

Pub. in Proceedings of the Defense Conference Nondestructive Testing (33rd), Morristown, New Jersey, November 27-29, 1984, p155-164 Aug 85.

Keywords: *Nondestructive tests, *Steels, Protective coatings, Corrosion, Organic coatings, Degradation, Reprints.

The authors have applied thermal-wave imaging, a recently-developed nondestructive technique, which is sensitive to minor variations in thermal conductivity of materials, and which can provide micrometer level resolution of subsurface features of opaque materials, to detect and assess degradation at the metal/coating interface. This paper will briefly review the technique of thermal-wave imaging and present preliminary results on the application of this method to imaging the corrosion of steel protected by organic coatings.

500,923

PB86-142890

Not available NTIS

National Bureau of Standards (NEL), Gaithersburg, MD. Building Materials Div.

Thermal-Wave Microscopy and Its Application to Imaging the Microstructure and Corrosion of Cold-Rolled Steel.

Final rept.,

T. Nguyen, and A. Rosencwaig. 1985, 18p

Pub. in Jnl. of Applied Surface Science 24, p57-74 1985.

Keywords: *Nondestructive tests, *Steels, Microscopy, Microstructure, Corrosion, Protective coatings, Reprints.

Thermal-wave microscopy (TWM), which employs heat flow to probe variations in the thermal properties of solid materials, can provide micron-level resolutions of subsurface features of opaque samples, this paper describes the principle of TWM, reviews its applications in material science, and presents the results of studies using this technique to imaging the microstructure and corrosion of cold-rolled steels. Preliminary results indicate that TWM can image the microstructure of cold-rolled steel with or without a corrosion layer. The results obtained also suggest that the technique can monitor and assess corrosion in its early stage of formation.

500,924

PB86-143740

Not available NTIS

National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.

Interlaboratory Comparison of Gold Thickness Measurements.

Final rept.,

F. Ogburn, and J. Mandel. 1985, 4p

Pub. in Plating and Surface Finishing 72, n9 p48-51 Sep 85.

Keywords: *Gold coatings, *Thickness, Dimensional measurement, Reprints.

Several factors contributed to the variability of gold thickness measurements during a round robin of 44 participating laboratories. The influence of individual factors and suggestions for improving the reliability of measuring the thickness of gold deposits with beta backscatter are presented.

500,925

PB86-165016

PC A04/MF A01

National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.

Fracture and Deformation: Technical Activities 1985.

Rept. for Oct 84-Oct 85,

R. P. Reed, and H. I. McHenry. Nov 85, 70p NBSIR-85/3189

Keywords: *Deformation, Research projects, Metals, Composite materials, Ceramics, Polymers, Fractures(Materials), *Fracture(Mechanics).

The report summarized the technical program of the Fracture and Deformation Division of the Institute for Materials Science and Engineering, National Bureau of Standards for the fiscal year 1985. The division's two major program areas are: elastic-plastic fracture mechanics and fracture mechanisms and analysis. Elastic-plastic fracture mechanics includes contributions from stress analysis, material properties, nondestructive-, and temperature- dependent properties, composite mechanics, and material performance comprise the second area, fracture mechanisms and analysis. Significant technical programs relating to each of these are presented. Major accomplishments are highlighted, including very successful dynamic crack arrest measurements using 10-m-long specimens, development of the dynamic theory of crack tip-dislocation interactions, and continued development and application of finite-element analysis and scattering theory for prediction of composite properties.

500,926

PB86-165032

PC A06/MF A01

National Bureau of Standards, Gaithersburg, MD. Inst. for Materials Science and Engineering.

Metallurgy Technical Activities, 1985,

E. N. Pugh, and J. G. Early. Nov 85, 116p NBSIR-85/3191

Keywords: *Metallurgy, Research projects, Microstructure, Mechanical properties, Wear, Corrosion, Electrodeposition, Nondestructive tests, Magnetic materials.

The report summarizes the FY1985 activities of the Metallurgy Division of the National Bureau of Standards. The research centers upon the structure-processing-properties relations of metals and alloys, and on the methods of their measurement. Task efforts comprise studies of synchrotron radiation research for materials characterization, metallurgical processing, wear and mechanical properties, chemical metallurgy, corrosion and protection of metals, electrodeposition, and nondestructive characterization. The work herein described includes three cooperative data programs with American professional societies and industry: the American Society for Metals-NBS Alloy Phase Diagram Program, the National Association of Corrosion Engineers-NBS Corrosion Data Program, and the American Iron and Steel Institute-NBS Steel Sensor Program. The scientific publications, invited talks, committee participation, and other professional interactions of the 91 full-time and part-time members of the Metallurgy Division and its 33 guest researchers are identified.

11G. Miscellaneous Materials

500,927

PB85-179059

(Order as PB85-179042, PC A06/MF A01)

National Bureau of Standards, Gaithersburg, MD. Center for Materials Science.

Indentation Fractography: A Measure of Brittleness,

B. R. Lawn, and D. B. Marshall. 30 Aug 84, 17p

Sponsored by Office of Naval Research, Arlington, VA. Prepared in cooperation with Rockwell International, Thousand Oaks, CA. Science Center.

Included in Jnl. of Research of the National Bureau of Standards, v89 n6 p435-451 Nov-Dec 84.

Keywords: *Fractography, *Brittleness, Crack propagation, Mechanical properties.

Indentation constitutes one of the most powerful test techniques for the systematic investigation of deformation and fracture responses in brittle materials. Indentations can be used to evaluate critical mechanical parameters (toughness, hardness, elastic modulus) with great simplicity and high accuracy.

11H. Oils, Lubricants, and Hydraulic Fluids

500,928

PB85-196103

Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

Development of an Oxidation-Wear Coupled Test for the Evaluation of Lubricants.

Final rept.,

R. S. Gates, and S. M. Hsu. 1984, 7p

Pub. in Lubrication Engineering 40, n1 p27-33 Jan 84.

Keywords: *Wear tests, *Oxidation, *Lubricants, *Degradation, Separation, Reprints.

Lubrication usually involves complex interactions between lubricant and metal surfaces under oxidizing conditions. The effects of lubricant degradation/oxidation on friction and wear are not well understood. Normal simulation of actual engine or bearing conditions usually examine wear and oxidation separately. Sometimes misleading conclusions are drawn. A thin-film micro-sample wear test has been developed using a four-ball wear tester in which the lubricant is subjected to oxidizing conditions and the time to seizure is measured. This measures both the friction and wear characteristics as well as the oxidation resistance of the lubricant. The test has been found useful in simulating ASTM engine sequence IIID wear test.

500,929

PB85-196178

Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

Lubrication Mechanism of SbSbS4.

Final rept.,

J. S. Harris, L. K. Ives, and M. B. Peterson. 1982, 2p Sponsored by Electron Microscopy Society of America, Oak Ridge, TN.

Pub. in Proceedings of Annual Meeting of the Electron Microscopy Society of America (40th), Washington, DC, August 9-13, 1982, p530-531.

Keywords: *Solid lubricants, *Lubricant additives, *Wear tests, Blends, Electron microscopy, Experimental design, *Antimony thioantimonate.

Recent laboratory investigations have reported that SbSbS4 is a promising solid lubricant when blended with several fluid lubricants. A series of different wear tests were conducted to determine the conditions and limits within which SbSbS4 functions as a lubricant. Results of these tests together with scanning and transmission electron microscopy analyses of worn surfaces on AISI 52100 steel were used to investigate the mechanism of lubrication. It was determined that SbSbS4 does not function as a solid lubricant at temperatures below about 225C. As an additive in lithium grease the lubricating mechanism of SbSbS4 is complex involving the formation of a solid film of SbSbS4 as well as the release of sulfur and its reaction with the steel surface.

500,930

PB86-111028

Not available NTIS

National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.

Evaluation of a New Wear Resistant Additive - SbSbS4.

Final rept.,

L. K. Ives, J. S. Harris, and M. B. Peterson. 1983, 7p Pub. in Proceedings of Wear of Materials, Reston, VA., April 11-14, 1983, p507-513.

Keywords: *Wear resistance, *Lubricant additives, *Greases, Electron microscopy, Performance evaluation, Lithium, *Antimony thioantimonate.

The addition of solid SbSbS4 powder to conventional lubricating base greases has been shown to result in reduced wear and a significant increase in load carrying capacity. In this investigation the antiwear behavior and response mechanisms of SbSbS4 when used as an additive to a lithium base grease are studied. Comparative block and ring tests were carried out on lithium base grease and on the base grease with separate additions of 5 wt% SbSbS4, and 0.43 wt% S. The tests were conducted under boundary lubrication conditions at a load of 267 N and a sliding speed of 5 cm/s utilizing 52100 steel specimen materials. Addition of 5 wt% SbSbS4 resulted in a reduction in wear rate by more than an order of magnitude compared to the base grease. The same effect, however, was achieved by the addition of 0.43 wt% S. This finding together with the identification of iron sulfide films on wear scar surfaces after lubrication with both SbSbS4 and S containing greases, indicated that the response of SbSbS4 was associated with the release of S and its reaction with the steel surface. The surface film studies described were carried out by means of analytical electron microscopy.

Field 11—MATERIALS

Group 11H—Oils, Lubricants, and Hydraulic Fluids

500,931

PB86-119344

Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Inorganic Materials Div.

Role of Iron and Copper in the Oxidation Degradation of Lubricating Oils.

Final rept.,
D. B. Clark, E. E. Klaus, and S. M. Hsu. 1985, 8p
Pub. in Lubrication Engineering 41, n5 p280-287 May 85.

Keywords: *Lubricating oils, *Oxidation, *Iron, *Copper, *Surface chemistry, Reaction kinetics, Metal containing organic compounds, Reprints, *Chemical reaction mechanisms.

In lubricant degradation, the role of metal surfaces in oxidation mechanisms has long been a subject of extensive study. In particular, copper and iron surfaces have been studied most frequently. However, data in the literature suggest both prooxidant and inhibiting characteristics for copper. A thin film microoxidation technique was used in this study to examine the role of copper and iron surfaces in the degradation process of lubricants. Metal analysis of the oxidized oil reveals that organometallic compounds are formed as a result of the lubricant-surface interactions. Different high-molecular-weight-reaction products from iron, copper, and glass result in varying effects on oxidation rates. This observation helps to explain the observed inhibiting effects and the prooxidant effects of copper in different systems. Iron has been found to promote oxidation much faster than copper.

500,932

PB86-138591

Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.

Solid Lubrication of Steel by SbSbS₄.

Final rept.,
L. K. Ives, and M. B. Peterson. 1984, 12p
Sponsored by Office of Naval Research, Arlington, VA. Pub. in Proceedings of Meeting of the Mechanical Failure Prevention Group (37th), Gaithersburg, Maryland, May 10-12, 1984, p208-219.

Keywords: *Solid lubricants, Steels, Antimony inorganic compounds, Antimonates, Friction, Wear, *Antimony thioantimonate.

The lubricating behavior of the amorphous solid, antimony thioantimonate (SbSbS₄), in the form of a dry powder and as compressed pellets is investigated and compared to MoS₂ and several other sulfides. The friction and wear response of the dry powders was determined by utilizing a three-pin-on-disk test configuration. Pins were of 52100 steel and disks were of 0-2 tool steel. Sliding experiments with compressed pellets of SbSbS₄, MoS₂, Sb₂S₃, FeS₂, and Fe_{0.9}S were used to study the friction, film forming, shear, and adhesion characteristics of the solid lubricant materials in the absence of metal to metal contact. A pin-on-ring configuration was employed with 52100 steel rings. The lubrication mechanism of SbSbS₄ is discussed on the basis of the results of these experiments. Simple models of solid film lubrication are presented to assist in the analysis.

11I. Plastics

500,933

PB85-187367

Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Chemical Engineering Science Div.

Thermal and Mechanical Properties of Polyurethane Foams at Cryogenic Temperatures.

Final rept.,
L. L. Sparks, and J. M. Arvidson. 1984, 14p
Sponsored by Gas Research Inst., Chicago, IL. Pub. in Proceedings of Society of the Plastics Industry (SPI) 28th Annual Technical/Marketing Conference, San Antonio, TX, November 5-7, 1984, p273-286.

Keywords: *Polyurethane resins, *Foam, *Thermal properties, *Mechanical properties, *Insulation, Cryogenics, Physical properties, Gas chromatography, Mass spectroscopy, Thermal expansion, *Expanded plastics.

Expanded plastics are used extensively for thermal insulation in cryogenic fuel facilities. Properties deter-

mined were thermal conductivity, thermal expansion, strength and moduli in compression and in tension, proportional limit, yield strength, ultimate strength, and shear strength. Physical properties were determined both parallel and perpendicular to the direction of foam rise. The gas content of the specimens was determined using a gas chromatograph-mass spectrometer, and the cell morphology was studied optically. Empirical procedures for estimating the temperature dependent thermophysical properties are discussed. These procedures utilize the characterization parameters for molar gas concentration and cell morphology.

500,934

PB85-222289

Not available NTIS
National Bureau of Standards, Gaithersburg, MD.

Solar Type Photolytic and Thermal Degradation of Plates of Polymethyl Methacrylate.

Final rept.,
B. Dickens, J. Martin, and D. Waksman. 1983, 2p
Pub. in Polymer Preprints, American Chemical Society, Division of Polymer Chemistry 24, n2 p84-85 1983.

Keywords: *Materials tests, *Polymethyl methacrylate, *Solar energy, *Thermal degradation, *Plates (Structural members), *Photolysis, Photochemical reactions, Oxidation, Polymerization, Temperature, Molecular structure, Photoplasticity, Plastics, Polymeric films, Reprints, Polymer chains, Chemical reaction mechanisms.

Specimens of 1.5 mm thick absorber-free PMMA containing about 1/2% monomer have been photolytically degraded in air at 50, 85 and 115°C and thermally degraded in air at 115 and 125°C. A simulated solar spectral range was used. Degradation was followed by GPC determinations of molecular weight as a function of depth in the specimen. The results show increased photo-degradation at the plate edges (back and front) over that occurring in the centers of the plates, and a rapidly attained constant amount of degradation for thermal degradation. The thermal degradation is ascribed to weak links, perhaps in-chain peroxides introduced during polymerization. The products of photo-oxidation absorb the shorter (300-320 nm) radiation significantly and progressively screen the remainders of the plate as degradation proceeds. Degradation mechanisms are proposed.

500,935

PB85-222388

Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Fire Measurement and Research Div.

Thermal and Oxidative Degradation of Poly(methyl methacrylate): Molecular Weight.

Final rept.,
T. Kashiwagi, T. Hirata, and J. E. Brown. Feb 85, 8p
Pub. in Macromolecules 18, n2 p131-138 Feb 85.

Keywords: *Polymethyl methacrylate, *Molecular weight, *Thermal degradation, *Oxidation tests, *Thermal analysis, Polymerization, Reaction kinetics, Reprints, *Chemical reaction mechanisms, *Thermal oxidation.

The mechanisms of thermal degradation and thermal oxidation of polymethylmethacrylate (PMMA) were studied by measuring the molecular weight of rapidly quenched samples thermally degraded in nitrogen and air in the range of temperatures between 200°C and 325°C. Results show that thermal oxidation reduces the degree of polymerization much faster than does thermal degradation. Random scission is the initiation step for both thermal degradation and oxidative degradation.

500,936

PB85-230001

Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.

Superposition of Small Strains on Large Deformations as a Probe of Nonlinear Response in Polymers.

Final rept.,
G. B. McKenna, and L. J. Zapas. 1985, 5p
Pub. in Proceedings of the SPE Annual Technical Conference and Exhibition (43rd), ANTEC 85, Plastics 85, p582-585 1985.

Keywords: *Plastic deformation, *Polyisobutylene, *Polymethyl methacrylate, *Strain measurement, *Mechanical tests, *Aging tests (Materials), Viscoelasticity, Solutions, Glass, Polymers, Nonlinear systems, *BKZ fluids, BKZ theory.

The incremental moduli, $\Delta G(+)$, for a concentrated solution of polyisobutylene (PIB) and for a PMMA

glass have been determined from step shear experiments in which a small deformation, ΔG , was superimposed upon a large deformation, γ (sub 1). $\Delta G(+)$ for both systems was found to decrease with increasing γ , and to increase with time, t (sub e), after the imposition of the large deformation. The results for the PIB are well described by the nonlinear constitutive equation of the BKZ elastic fluid theory. However, the polymer glass shows less nonlinearity than predicted by the BKZ theory. The results are used to show the ambiguity of molecular interpretations from these types of experiments.

500,937

PB85-230829

Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymer Science and Standards Div.

Creep and Stress-Relaxation Behavior of Ultra High Molecular Weight Polyethylene in Uniaxial Extension and Compression.

Final rept.,
J. M. Crissman, G. B. McKenna, and F. Khoury. 1982, 5p
Sponsored by Society of Plastic Engineers, Brookfield Center, CT.

Pub. in Proceedings of ANTEC/82, Annual Technical Conference and Exhibition of the Society of Plastics Engineers (40th): Plastics - Meeting Challenges of the Future, San Francisco, California, May 10-13, 1982, p55-58.

Keywords: *Molecular relaxation, *Creep tests, *Stress relaxation tests, *Polyethylene, *Compression tests, Molecular weight, Morphology, Mechanical properties, Plastics, Cold flow.

The manuscript represents the text of a paper which will be presented at the 40th Annual ANTEC sponsored by the Society of Plastics Engineers. The work described in the abstract is concerned with a study of the relationship of morphology to the mechanical behavior of ultra high molecular weight polyethylene (UHMWPE) used in the manufacture of orthopedic prostheses, and it is being done under contract with the Food and Drug Administration, Bureau of Medical Devices. Both the morphology and mechanical behavior have been studied for samples of UHMWPE prepared under widely different processing conditions. Two results of significance are (1) that in uniaxial extension deformation of the material does not occur uniformly on a microscopic scale, rather it reflects the particulate nature of the raw polymer powder, and (2) that small changes in the crystallinity of the material can significantly alter the creep and stress-relaxation behavior. It is also shown that the environmental stress-crack resistance of UHMWPE is highly dependent upon the thermal history given compression molded samples.

500,938

PB86-111788

Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD.

Study of Oxygen Effects on Nonflaming Transient Gasification of PMMA and PE during Thermal Irradiation.

Final rept.,
T. Kashiwagi, and T. J. Ohlemiller. 1982, 9p
Sponsored by Combustion Inst., Pittsburgh, PA. Pub. in Proceedings of Symposium on Combustion (19th), Haifa, Israel, August 8-13, 1982, p815-823.

Keywords: *Oxygen, *Polymethyl methacrylate, *Polyethylene, *Gasification, *Thermal degradation, *Surface chemistry, Pyrolysis, Oxidation, Nitrogen, Mixture, *Low density polyethylene.

The effects of gas phase oxygen on the rate of gasification and surface temperature history of large samples of PMMA and low density PE were investigated under transient, nonflaming heating by thermal radiation. Four different ambient gas mixtures, nitrogen, 10% O₂/90% N₂, 20% O₂/80% N₂, and 40% O₂/60% N₂, were used. Two different radiant fluxes, 1.7 and 4.0 W/sq cm, were used. For PMMA, large bubbles are formed in the hottest, near-surface layer in a nitrogen environment; these bubbles are smaller and more frequent in oxygen-containing environments. An increase in oxygen concentration significantly decreases the surface temperature of PMMA and even more significantly increases that with PE.

500,939

PB86-113644

Not available NTIS

National Bureau of Standards, Gaithersburg, MD. Polymer Science and Standards Div.

Deformation and Failure of Ultra High Molecular Weight Polyethylene.

Final rept.,
G. B. McKenna, J. M. Crissman, and F. Khoury.
1981, 3p

Sponsored by Food and Drug Administration, Silver Spring, MD. Bureau of Medical Devices.

Pub. in Proceedings of the Society of Plastics Engineers Annual Technical Conference and Exhibition (39th) on Plastics - Creating Value Through Innovation, Boston, MA., May 4-7, 1981, p82-84.

Keywords: *Polyethylene, *Deformation, *Failure analysis, Molecular weight, Stress relaxation, Creep tests, Plastics.

In this paper the authors report results from a study of the effects of morphology/processing on the time dependent mechanical behavior of UHMWPE. To date, the creep and stress relaxation behaviors in uniaxial extension have been examined for compression molded sheets which have been either slowly cooled or quenched from the melt. In addition, results are reported for the failure behavior in constant load (creep), and sinusoidal loading (fatigue) conditions for the polymer which has been slowly cooled from the melt. At the same time the morphologies of both the raw polymer and compression molded sheets have been examined.

500,940

PB86-130150

Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymer Science and Standards Div.

Small-Angle Neutron-Scattering of Partially Segregated Blends of Polyethylene and Deuteropolyethylene.

Final rept.,
W. Wu, and G. D. Wignall. 1985, 6p
Pub. in Polymer 26, n5 p661-666 1985.

Keywords: *Polyethylene, *Deuterium compounds, Melting, Crystallization, Neutron scattering, Plastic deformation, Comparison, Sampling, Molecular weight, Substitutes, Neutron scattering, Temperature, Mathematical models, Reprints, *Small angle scattering, Chemical reaction mechanisms.

In previous paper, polyethylene (PEH) blended with 4.3 vol % deuterated polyethylene (PED) was annealed and plastically deformed at different temperatures. The most prominent change resulting from the deformation is a significant reduction in the apparent molecular weight measured from the extrapolated small-angle neutron scattering (SANS) data. The model adopted in the data interpretation was based on a heterogeneous distribution of the centers of mass of the labeled (PED) chains which form a two phase system of enriched and depleted regions described by a Debye like correlation function. A comparison between this model and alternative approaches based on the correlation network and random phase approximation will be delineated. The results from these models lead to the conclusion that for typical melt crystallized samples the centers of mass of the labeled chains are only slightly perturbed from a random distribution. Plastic deformation of the blends tends to lessen the degree of segregation of the PED molecules and the results suggest that a portion of the specimen must undergo a melting and recrystallization mechanism during deformation.

500,941

PB86-133501

Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymer Science and Standards Div.

Thermodynamic Properties and Glass-Transition of Polystyrene.

Final rept.,
S. S. Chang. 1984, 18p
Pub. in Jnl. of Polymer Science-Polymer Symposia Edition, n71 p59-76 1984.

Keywords: *Polystyrene, *Thermodynamic properties, *Glass transition temperature, Specific heat, Molecular weight, Heat capacity, Reprints, Standard reference material.

Heat capacity of a narrow molecular weight distribution polystyrene, National Bureau of Standards-Standard Reference Material 1478, has been determined by a fully automated adiabatic calorimeter from 5 to 380 K for the sample subjected to different thermal history. The number-average molecular weight of this sample

is 35,800 and the dispersity in the molecular weights, $M(\text{sup w}):M(\text{sup n})$ is 1.045. The heat capacity of the glass and of the liquid of this material are found to be within 0.5% of other atactic polystyrenes over most of the temperature range studied.

500,942

PB86-136769

Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymer Science and Standards Div.

Thermal and Photolytic Degradation of Plates of Poly(methyl methacrylate) Containing Monomer.

Final rept.,
B. Dickens, J. W. Martin, and D. Waksman. 1984, 10p
Pub. in Polymer 25, n5 p706-715 1984.

Keywords: *Polymethyl methacrylate, *Degradation, *Thermal analysis, Oxidation, Photochemical reactions, Plates (Structural members), Temperature, Reprints, Monomers, Chemical reaction mechanisms.

Specimens of 1.5 mm thick absorber-free PMMA containing about 0.5 percent monomer have been photolytically degraded in air at 50, 85, and 115 C and thermally degraded in air at 115 and 125 C. Specimens were exposed to a simulated solar spectral range. Degradation was followed by GPC determinations of molecular weight as a function of depth in the specimens. The results show increased photo-degradation at the plate edges (back and front) over that occurring in the centers, and a rapidly attained constant amount of degradation for thermal degradation. The effect of temperature is mostly to decrease the importance of the cage effect and to allow the initial radicals formed to diffuse away from one another. The products of photo-oxidation absorb the shorter (300 to 330 micrometers) radiation significantly and progressively screen the remainder of the plate as degradation proceeds. Degradation mechanisms are proposed.

500,943

PB86-151941

PC E17/MF E17
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.

Review of the Literature on the Gaseous Products and Toxicity Generated from the Pyrolysis and Combustion of Rigid Polyurethane Foams.

M. Paabo, and B. C. Levin. Dec 85, 113p NBSIR-85/3224

Sponsored by Consumer Product Safety Commission, Bethesda, MD.

Keywords: *Urethane resins, *Pyrolysis, *Flammability testing, *Air pollution, *Toxicity, Reviews, Combustion products, Foam, Biochemistry, Carbon monoxide, Hydrogen cyanide, Dosage, Indoor air pollution, Consumer products.

The literature on rigid polyurethane foam has been reviewed with an emphasis on the gaseous products generated under various thermal decomposition conditions and the toxicity of those products. The review is limited to publications in English through 1984. Carbon monoxide (CO) and hydrogen cyanide (HCN) were the predominant toxicants found among more than 100 other gaseous products. The generation of CO and HCN was found to increase with increasing combustion temperatures. Many test methods were used to assess the acute inhalation toxicity of combustion products from various rigid polyurethane foams. Lethality, incapacitation, physiological, and biochemical parameters were employed as biological end points. In general, the combustion products generated from rigid polyurethane foam in the flaming mode appear to be more toxic than those produced in the non-flaming mode. The LC50 values for 30 minute exposures ranged from 10 to 17 mg/l in the flaming mode and were greater than 34 mg/l in the nonflaming mode. With the exception of one case in which a reactive type phosphorus containing fire retardant was used, the addition of fire retardants to rigid polyurethane foams does not appear to generate unusual toxic combustion products.

11J. Rubbers

500,944

PB85-189306

Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.

Failure Behavior of Rubber-Toughened Epoxies in Bulk, Adhesive, and Composite Geometries.

Final rept.,
D. L. Hunston, and W. D. Bascom. 1984, 17p
Prepared in cooperation with Naval Research Lab., Washington, DC. Chemistry Div.
Pub. in ACS (American Chemical Society) Advances in Chemistry Series, n208 p83-99 1984.

Keywords: *Rubber adhesives, *Composite materials, *Epoxy resins, *Failure, Temperature, Viscoelasticity, Reprints.

Rubber-modified epoxies were first developed empirically in the 1960's to improve the poor crack-growth resistance of epoxies with a minimum sacrifice in other desirable properties. In 1971 a major effort was launched to study the failure behavior of these materials as structural adhesives. Since then, this program has been expanded to include numerous laboratories and researchers, and the objectives have been broadened to include the failure behavior of bulk specimens and fiber-reinforced composites as well. The authors discuss the effects on failure behavior of rubber modification, test temperature, and loading rate for all three specimen types. For adhesive bonds, the effects of bond thickness are also discussed.

500,945

PB85-202588

Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Experiments on the Small Strain Behavior of Crosslinked Natural Rubber. 2. Extension and Compression.

Final rept.,
G. B. McKenna, and L. J. Zapas. 1983, 5p
See also PB85-104750.
Pub. in Polymer 24, n11 p1502-1506 Nov 83.

Keywords: *Natural rubber, *Strain tests, Experimental design, Crosslinking, Compressing, Modulus of elasticity, Extensions, Tension tests, Elastomers, Reprints.

Experiments were carried out to characterize the small strain tension and compression behavior of dicumyl peroxide crosslinked natural rubber. Strains which were smaller by an order of magnitude than any reported previously on natural rubber were achieved. The authors results support the contention that the compression and extension moduli of natural rubber are different. A new finding is reported. That is, the moduli in tension and compression do not become constant but rather they increase significantly as zero deformation is approached.

500,946

PB85-204717

PC A06/MF A01
National Bureau of Standards, Gaithersburg, MD.
Structure and Properties of Polyethylene Films Used in Heavy Lift Balloons.

Rept. for Jan-May 84,
F. Khoury, J. M. Crissman, B. M. Fanconi, H. L. Wagner, and L. H. Bolz. Mar 85, 105p NBSIR-84/2989-NASA
Sponsored by National Aeronautics and Space Administration, Wallops Island, VA. Wallops Flight Center.

Keywords: *Polyethylene, *Polymeric films, *Mechanical properties, *Balloons, Molecular weight, Melting point, Density(Mass/volume), Surface properties, Birefringence, Graphs(Charts), Tensile properties, X ray diffraction, Crystal structure, Morphology, Strain rate, Infrared spectroscopy, Fine structure, Fourier transform spectroscopy, Polymer branching, Polymer chains.

The following features of five polyethylene films used by NASA in the construction of heavy lift balloons have been examined: molecular weight, molecular weight distribution, branching, melting behavior, density, surface texture, birefringence, orientation of crystalline regions, uniaxial deformation in the machine and transverse directions, and the effect of sample geometry and strain rate on deformation behavior. The goal of this exploratory study was to determine whether there are significant differences in any of the above mentioned features, or combination of features between the films. The acquisition of such information is a first step towards determining whether there are any specific correlations between film characteristics and the incidence of catastrophic failure of balloons during ascent through the troposphere. This exploratory study has resulted in the identification of similarities and differences between various features of the films. Close similarities have been found in methyl group content, crystallinity, and peak melting temperature.

Field 11—MATERIALS

Group 11J—Rubbers

The preferred orientations in the crystalline regions appear to be qualitatively similar or related. Differences among the films have been revealed in two features, namely between their molecular weights, and in the balance of the strain to break behavior in the machine direction relative to that in the transverse direction.

500,947

PB86-142858

Not available NTIS

National Bureau of Standards, Gaithersburg, MD. Polymers Div.

Superposition of Small Deformations on Large Deformations: Measurements of the Incremental Relaxation Modulus for a Polyisobutylene Solution.

Final rept.,

G. B. McKenna, and L. J. Zapas. 1985, 10p

Pub. in Jnl. of Polymer Science, Polymer Physics Edition 23, p1647-1656 1985.

Keywords: *Modulus of elasticity, *Molecular relaxation, *Deformation, Solutions, Viscoelasticity, Aging tests(Materials), Elastomers, Reprints, *Polyisobutylene, BKZ theory.

The incremental relaxation modulus $\delta G(t)$ for a concentrated solution of polyisobutylene has been determined from step-shear experiments in which a small deformation $\delta\gamma$ was superimposed on a large deformation γ_1 ; $\delta G(t)$ was found to decrease with increasing γ_1 , and to increase with the t after the imposition of the large deformation. It was also observed that the 'apparent relaxation spectrum' associated with $\delta G(t)$ narrows and shifts to shorter times when compared to the spectrum associated with the linear viscoelastic relaxation modulus $G(t)$. The results are well described by the nonlinear constitutive equation of the BKZ elastic fluid theory.

The paper presents computational procedures for generating bounds on measures of network reliability. The two measures considered, reachability and connectedness, are the probability that there is an operating path from a node to all other nodes in a directed (respectively undirected) stochastic network. The bounds, which are given in terms of polynomials in p , the common arc failure probability, are based on recent bounding results the authors developed for the class of shellable independence systems. Two pairs of bounds are given weaker bounds whose computation time is bounded by a polynomial in the size of the network and tighter bounds whose computation time is bounded by a polynomial in the size of the network and the number of minimum cardinality network cuts. Computational results are also given that evaluate the quality of the bounds. The generation of the bounds involves several interesting path and cut counting problems.

500,950

PB85-189496

Not available NTIS

National Bureau of Standards (NEL), Gaithersburg, MD. Scientific Computing Div.

Solving Elliptic Problems Using ELLPACK.

Final rept.,

J. R. Rice, and R. F. Boisvert. 1985, 497p

Prepared in cooperation with Purdue Univ., Lafayette, IN.

Pub. in Proceedings of Solving Elliptic Problems Using ELLPACK 2, 497p 1985.

Keywords: *Partial differential equations, *Elliptic differential equations, *Boundary value problems, Finite difference theory, Finite element analysis, Numerical integration, Linear differential equations, Reprints, *ELLPACK system, Two dimensional calculations, Three dimensional calculations, Computer software.

This book describes the use of the ELLPACK system and language for solving elliptic boundary value problems. ELLPACK provides many facilities for solving two-dimensional, linear elliptic partial differential equations on rectangular domains, and several facilities for non-rectangular domains and for three-dimensional rectangular domains. The book includes a users guide, a module reference, a contributors guide, and a system programmers guide.

500,951

PB85-197440

Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

Random Walk on a Random Channel with Absorbing Barriers.

Final rept.,

D. A. Huckaby, and J. B. Hubbard. 1983, 9p

Pub. in Physica A 122, n3 p602-610 Dec 83.

Keywords: *Random walk, *Diffusion theory, *Membranes, Absorbers(Materials), Barriers, Reprints.

The authors investigate a random walk which takes place on a one dimensional random channel, where both walker and channel are confined by absorbing barriers. The authors are able to analytically follow the transition from diffusive to non-diffusive behavior as the minimum number of channel segments required to traverse the membrane increases.

500,952

PB85-197507

Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

Program to Simulate the Galton Quincunx.

Final rept.,

J. Hilsenrath, and B. F. Field. 1983, 3p

Pub. in Math. Teacher 76, n8 p571-573 Nov 83.

Keywords: *Normal density functions, *Computer programs, BASIC programming language, Computerized simulation, Reprints, *Galton quincunx.

A BASIC program is presented and described which produces a normal distribution on the computer screen in the manner of a Galton Quincunx.

500,953

PB85-201937

Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

Determinacy in Linear-Systems and Networks.

Final rept.,

J. S. Provan. 1983, 17p

Pub. in SIAM (Society for Industrial and Applied Mathematics) Jnl. of Algebraic Discrete Meth. 4, n2 p262-278 1983.

Keywords: *Linear systems, *Networks, Correlations, Transportation, Reprints, Sensitivity analysis.

Interdependent and determinate behavior is studied between variables subject to a system of linear equalities. For each pair of variables in such a system, four definitions of 'correlation' are introduced which relate the behavior of the variables to a chosen set of 'basic' variables for the system. These definitions correspond directly to such terms as statistical correlation, rates of substitution in economics, sensitivity in linear programming, and sign-solvability in linear algebra. For each definition of correlation, there is a stronger property of determinacy between two variables, established by the consistency in sign of the correlation between the two variables over every set of basic variables. The authors show that the property of determinacy is independent of which definition of correlation is used. The author also examines correlation and determinacy in systems related to networks, and derive good characterizations of determinacy in terms of properties of the underlying networks.

500,954

PB85-202810

Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

New Statistic for Detecting Influential Observations in a Scheffe' Type Calibration Curve.

Final rept.,

C. H. Spiegelman. Dec 84, 8p

Pub. in Australian Jnl. of Statistics 26, Part 3 p290-297 Dec 84.

Keywords: *Calibrating, *Statistics, Reprints.

A statistic for identifying influential observations in calibration is given. The statistic is easy to interpret, and provides a useful measure of influence for Scheffe' type calibration curves.

500,955

PB85-205714

Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

Invariance of Perturbed Null Vectors under Column Scaling.

Final rept.,

G. W. Stewart. 1984, 5p

Pub. in Numerische Mathematik 44, n1 p61-65 1984.

Keywords: *Matrices(Mathematics), Perturbation theory, Invariance, Reprints.

Let X be an $n \times p$ matrix of rank $p-1$, and let u be a null vector of X . If T is nonsingular and v' is a suitably scaled null vector of $X = XT$, then $v = Tv'$. Now let $(X \text{ tilde}) = X + E$ and $(x \text{ tilde})' = (X \text{ tilde})T$. It is shown that if $(v \text{ tilde})$ and $(v \text{ tilde})'$ are singular vectors of $(X \text{ tilde})$ and $(X \text{ tilde})'$ corresponding to their smallest singular values, then $(v \text{ tilde}) = T(v \text{ tilde})' + O(11E^{11} \text{ sup } 2)$.

500,956

PB85-208148

Not available NTIS

National Bureau of Standards (NEL), Gaithersburg, MD. Mathematical Analysis Div.

Inverse Gaussian Pulse in the Experimental Determination of Linear System Green's Functions,

S. Carasso, and N. Hsu. Feb 85, 16p

Sponsored by Army Research Office, Research Triangle Park, NC.

Pub. in Transactions of the Second Army Conference on Applied Mathematics and Computing, Troy, New York, May 1984, ARO Report 85-1, p389-404 Feb 1985.

Keywords: *Greens function, Linear systems, Time invariant systems, Acoustic emissions, Deconvolution, Impulse response.

A new time domain deconvolution method is presented for determining the 'impulse response' of linear time invariant systems. The method is based on the use of the one-sided, causal, inverse Gaussian pulse as an approximation to the Dirac delta-function. Deconvolution of that kernel is equivalent to an inverse heat conduction problem. The method is particularly useful in cases where the Green's function for the linear system has singularities such as jumps, cusps, spikes, and the like. Computational reconstructions of singularities, from smooth synthetic data, are presented in the context of Acoustic Emission Green's functions.

12. MATHEMATICAL SCIENCES

12A. Mathematics and Statistics

500,948

PB85-182699

Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

Ideal Resonance Problem at First Order.

Final rept.,

A. Deprit. 1982, 6p

Sponsored by American Astronautical Society, Alexandria, VA., and American Inst. of Aeronautics and Astronautics, New York.

Pub. in Proceedings of AAS/AIAA Astrodynamics Conference, North Lake Tahoe, NV, August 3-5, 1981, Advances in the Astronautical Sciences, v46 p521-526 1982.

Keywords: *Resonance, *Oscillation, Elliptic functions, Perturbation theory, Pendulums, Nonlinear systems.

Perturbations of the first order are removed jointly by a canonical transformation representing the hunting effect, and by a change of the time to synchronize the perturbed pendulum. Both operations are expressed in elementary functions. The reduced system is a simple pendulum integrable by elliptic functions.

500,949

PB85-183184

Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

Calculating Bounds on Reachability and Connectedness in Stochastic Networks.

Final rept.,

M. O. Ball, and J. S. Provan. 1983, 26p

Pub. in Networks 13, n2 p253-278 1983.

Keywords: Algorithms, Approximation, Graphics, Networks, Probability theory, Reliability, Reprints, *Stochastic networks.

500,957
PB86-103587 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Mathematical Analysis Div.
Probe Waveforms and Deconvolution in the Experimental Determination of Elastic Green's Functions.
Final rept.,
A. S. Carasso, and N. N. Hsu. Jun 85, 14p
Contract ARO-63-82
Pub. in SIAM (Society for Industrial and Applied Mathematics) Jnl. on Applied Mathematics 45, n3 p369-382 Jun 85.

Keywords: *Signal processing, Greens function, Linear systems, Cauchy problem, Reprints, *Impulse response, Acoustic emissions, Initial value problems, Deconvolution.

The authors propose a new time domain method for the experimental determination of the 'impulse response' of linear systems. The technique centers around the use of specifically designed probe waveforms. These w unit step function, and lead to a subsequent time domain deconvolution problem which can be implemented as a Cauchy initial value problem. This approach allows for continuous deconvolution, a powerful option in the presence of noise. The authors orient the discussion to the context of acoustic emission and elastic Green's functions, and present several numerical reconstructions of sharp signals from smooth synthetic data.

500,958
PB86-103645 Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Statistical Engineering Div.
Computational Experience with Confidence Regions and Confidence Intervals for Nonlinear Least Squares.
Final rept.,
J. R. Donaldson, and R. B. Schnabel. May 85, 30p
Pub. in University of Colorado Department of Computer Science Technical Report CU-CS-302-84, 30p May 85.

Keywords: *Least squares method, Monte Carlo method, Confidence limits, Computation, *Parameter estimation, Nonlinear analysis, Linearization.

The authors present the results of a Monte Carlo study of the most commonly discussed methods for constructing approximate confidence regions and confidence intervals for parameters estimated by nonlinear least squares. The methods examined are the three variants of the linearization method, the likelihood method, and the lack-of-fit method. The linearization method is the most frequently implemented method. It is computationally inexpensive and produces easily understandable results. The likelihood and lack-of-fit methods both are much more expensive and more difficult to report. Based on results, it is concluded that among the three variants of the linearization method, the variant based solely on the Jacobian appears preferable because it is simple, less expensive, more numerically stable, and at least as accurate as the other two variants which utilize the full Hessian.

500,959
PB86-112083 Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Scientific Computing Div.
Successive Overrelaxation, Multigrid, and Preconditioned Conjugate Gradients Algorithms for Solving a Diffusion Problem on a Vector Computer.
Final rept.,
J. Gary, S. McCormick, and R. Sweet. 1983, 25p
Pub. in Proceedings of International Conference on Multigrid Methods, Dillon, CO., April 6-8, 1983, Applied Mathematics and Computation 13, n3/4 p285-309 1983.

Keywords: *Diffusion theory, Elliptic differential equations, Matrices(Mathematics), Numerical integration, Algorithms, *Successive overrelaxation method, *Multigrid methods, *Conjugate gradient method, Vector processors.

The purpose of the paper is the treatment of three numerical algorithms (successive overrelaxation (SOR), multigrid (MG) and conjugate gradients preconditioned by a fast Poisson solver (CG)) for solving large but mildly behaved diffusion problems on a vector comput-

er with memory-to-memory architecture. The problem is a symmetric nonnegative definite matrix equation arising from a cell-centered finite difference approximation of a 3-d diffusion equation with full Neumann boundary conditions.

500,960
PB86-128956 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Mathematical Analysis Div.
Decay of Solutions of Wave-Equations in a Bounded Region with Boundary Dissipation.
Final rept.,
J. Lagnese. 1983, 20p
Pub. in Jnl. of Differential Equations 50, n2 p163-182 1983.

Keywords: *Wave equations, Energy dissipation.

An energy decay rate is obtained for solutions of the wave equation in a bounded region in $(R \supset \eta)$ whose boundary consists partly of a nontrapping reflecting surface and partly of an energy absorbing surface.

500,961
PB86-132537 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Operations Research Div.
Banach-Spaces That Have Normal Structure and Are Isomorphic to a Hilbert-Space.
Final rept.,
J. Bernal, and F. Sullivan. 1984, 5p
Pub. in Proceedings of American Mathematical Society 90, n4 p550-554 1984.

Keywords: *Banach space, Hilbert space, Reprints.

The authors prove that given a Hilbert space $(E, \langle \cdot, \cdot \rangle)$, and $\langle \cdot, \cdot \rangle$ a norm on E such that for all x ϵ E , $1/\beta \langle x, x \rangle = \langle x, x \rangle$ or $\langle x, x \rangle = \langle x, x \rangle$ for some β , if $1 = \langle x, x \rangle < \beta < (\text{square root of } 2)$, then $(E, \langle \cdot, \cdot \rangle)$ satisfies a convexity property from which normal structure follows.

500,962
PB86-138344 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Statistical Engineering Div.
Notched Box-and-Whisker Plot.
Final rept.,
K. Kafadar. 1985, 4p
Pub. in Encyclopedia of Statistical Sciences, v6 p367-370 1985.

Keywords: *Statistical analysis, Statistical tests, Significance.

A statistical article is to be submitted to the Encyclopedia of Statistical Sciences. Definitions and applications are given for each entry.

500,963
PB86-138377 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Scientific Computing Div.
Sources of Information on Quadrature Software.
Final rept.,
D. Kahaner. 1984, 31p
Pub. in Sources and Development of Mathematical Software, ch7 p134-164 1984.

Keywords: *Numerical quadrature, *Integral equations, Computer software.

The paper surveys the area of numerical quadrature - evaluation of integrals. Particular emphasis is placed on the problems which lend themselves to efficient solution by readily available computer programs from four well supported libraries. The authors describe several of the basic ideas now in use and point out software built upon them. The paper assumes very little background in quadrature. It is not a complete tutorial on quadrature but does hope to give a few salient details.

500,964
PB86-142841 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Applied Mathematics.
National Bureau of Standards.
Final rept.,
J. R. Rosenblatt. 1985, 3p
Pub. in Encyclopedia of Statistical Sciences, v6 p148-150 1985.

Keywords: *Statistical analysis, Measurement, Test methods.

The article provides a brief description of statistical aspects of the work of the National Bureau of Standards.

500,965
PB86-165792
(Order as PB86-165776, PC A08/MF A01)
National Bureau of Standards, Gaithersburg, MD.
Jack Youden,
H. H. Ku, and J. R. DeVoe. Dec 85, 2p
Included in Jnl. of Research of the National Bureau of Standards, v90 n6 p393-394 Nov-Dec 85.

Keywords: Chemist, Statistical analysis, Chemical analysis, *Youden Jack, Statisticians.

Jack Youden was a chemist and a communicator. The Chemical Division of the American Society for Quality Control in 1969 established a Jack Youden prize to be awarded yearly for the best expository paper in its journal, Technometrics. But it was Youden the statistician who furthered collaboration and helped to maximize the information content of experimentation, which is what the Chemometrics Conference was about. So it appropriate that these conference proceedings be dedicated to the memory of Dr. Youden.

500,966
PB86-165826
(Order as PB86-165776, PC A08/MF A01)
Washington State Univ., Pullman.
Adaptive Kalman Filtering,
S. D. Brown, and S. C. Rutan. 24 Jun 85, 5p
Prepared in cooperation with Virginia Commonwealth Univ., Richmond. Sponsored by National Bureau of Standards, Gaithersburg, MD.
Included in Jnl. of Research of the National Bureau of Standards, v90 n6 p403-407 Nov-Dec 85.

Keywords: *Chemical analysis, Least squares method, Data reduction, Covariance, *Kalman filtering, Computer applications.

The increased power of small computers makes the use of parameter estimation methods attractive. Such methods have a number of uses in analytical chemistry. When valid models are available, many methods work well, but when models used in the estimation are in error, most methods fail. Methods based on the Kalman filter, a linear recursive estimator, may be modified to perform parameter estimation with erroneous models. Modifications to the filter involve allowing the filter to adapt the measurement model to the experimental data through matching the theoretical and observed covariance of the filter innovations sequence. The adaptive filtering methods that result have a number of applications in analytical chemistry.

500,967
PB86-165883
(Order as PB86-165776, PC A08/MF A01)
National Bureau of Standards, Gaithersburg, MD.
Regression Analysis of Collinear Data,
J. Mandel. 1 Jul 85, 14p
Included in Jnl. of Research of the National Bureau of Standards, v90 n6 p465-478 Nov-Dec 85.

Keywords: *Regression analysis, *Chemical analysis, Measurement, Collinearity.

The paper presents a technique based on the intuitively-simple concepts of Sample Domain and Effective Prediction Domain, for dealing with linear regression situations involving collinearity of any degree of severity. The Effective Prediction Domain (EPD) clarifies the concept of collinearity, and leads to conclusions that are quantitative and practically useful. The method allows for the presence of expansion terms among the regressors, and requires no changes when dealing with such situations.

500,968
PB86-165917
(Order as PB86-165776, PC A08/MF A01)
Wisconsin Univ.-Madison.
Some New Ideas in the Analysis of Screening Designs,
G. Box, and R. D. Meyer. 1 Jul 85, 8p
Included in Jnl. of Research of the National Bureau of Standards, v90 n6 p495-502 Nov-Dec 85.

Keywords: *Experimental design, Screenings, *Factorial design.

Consideration of certain aspects of scientific method leads to discussion of recent research on the role of

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screening designs in the improvement of quality. A projective rationale for the use of these designs in the circumstances of factor sparsity is advanced. In this circumstance the possibility of identification of sparse dispersion effects as well as sparse location effect is considered. A new method for the analysis of fractional factorial designs is advanced.

500,969

PB86-165966

(Order as PB86-165776, PC A08/MF A01)
Columbia Univ., New York.

Regression Analysis of Compartmental Models,

T. L. Lai. 24 Jun 85, 6p

Sponsored by National Bureau of Standards, Gaithersburg, MD.

Included in Jnl. of Research of the National Bureau of Standards, v90 n6 p525-530 Nov-Dec 85.

Keywords: *Regression analysis, *Mathematical models, *Compartment analysis, Least squares method, Decay, Kinetics, System identification.

Herein the authors study the problem of assessing, on the basis of noisy and incomplete observations, how much information there is in the data for model identification in compartmental systems. The underlying concept is that of an 'information distance' between competing models, and estimation of this distance on the basis of the given data is discussed. Useful reduction of the dimensionality of the corresponding least squares problem is accomplished by regarding the decay rate constant as primary parameters of interest and the other parameters of the model as nuisance parameters. Estimation of the decay rate function is also discussed.

12B. Operations Research

500,970

PB85-201986

Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

Computing Network Reliability in Time Polynomial in the Number of Cuts.

Final rept.,

J. S. Provan, and M. O. Ball. 1984, 11p

Pub. in Operations Research 32, n3 p516-526 1984.

Keywords: *Networks, Computation, Reliability, Polynomials, Algorithms, Reprints, *Stochastic networks, Probability.

In this paper, the authors present a new algorithm for computing the probability that there exists an operating path from a node s to a node t in a stochastic network. This algorithm has the special property that computation time is bounded by a polynomial in the number of (s,t) -cuts in the network. They also investigate other connectedness reliability problems in terms of their complexity with respect to the number of cut-sets and pathsets in the network. They indicate which problems do have algorithms which are polynomial in the number of such sets, and which ones will not have such algorithms unless $P=NP$.

500,971

PB86-105830

Not available NTIS

National Bureau of Standards (NEL), Gaithersburg, MD. Scientific Computing Div.

Family of Descent Functions for Constrained Optimization.

Final rept.,

P. T. Boggs, and J. W. Tolle. Dec 84, 16p

Grant DAAG29-77-G-0125

Sponsored by Army Research Office, Research Triangle Park, NC.

Pub. in SIAM (Society for Industrial and Applied Mathematics) Jnl. on Numerical Analysis 21, n6 p1146-1161 Dec 84.

Keywords: *Nonlinear programming, Convergence, Algorithms, Reprints, *Constrained optimization.

In order to achieve a robust implementation of methods for nonlinear programming problems, it is necessary to devise a procedure which can be used to test whether or not a prospective step would yield a 'better' approximation to the solution than the current iterate. In this paper, the authors present a family of descent or merit functions which are shown to be compatible with local Q-superlinear convergence of Newton and

quasi-Newton methods. A simple algorithm is used to verify that good descent and convergence properties are possible using this merit function.

500,972

PB86-105988

PC A03/MF A01

National Bureau of Standards (NEL), Gaithersburg, MD. Center for Applied Mathematics.

Global Solutions to Factorable Nonlinear Optimization Problems Using Separable Programming Techniques,

G. P. McCormick. Jul 85, 46p NBSIR-85/3206

Keywords: *Mathematical programming, Least squares method, Computation, Optimization, Algorithms, Nonconvex programming, Branch and bound method, Nonlinear analysis.

Many algorithms for obtaining global solutions to non-convex optimization problems have been proposed in recent years. The methods farthest along computationally are those for separable problems. These use linear programming codes to solve sequences of LP problems formed from piece-wise linear approximations to the nonlinear functional forms. For a large class of optimization problems, called factorable programming problems, it is possible to create equivalent separable problems. This is done at a cost: additional variables and constraints. In this paper the procedure for creating the equivalent separable problems is outlined and a brief description is given of a global solution algorithm due to Falk. A small example is given illustrating the above techniques. The example is also solved using a more direct method. Application to the solution of nonlinear least squares is illustrated with another example. Discussion of areas of research for improving the efficiency of this approach concludes the paper.

500,973

PB86-119203

Not available NTIS

National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.

Characterizing Supremum and I (sub p) Efficient Facility Designs.

Final rept.,

L. G. Chalmet, R. L. Francis, and J. F. Lawrence.

1981, 13p

See also AD-A059040. Sponsored by Army Research Office, Research Triangle Park, NC., and National Research Council, Washington, DC.

Pub. in Jnl. of Optimization Theory and Applications 35, n1 p129-141 Sep 81.

Keywords: *Experimental design, *Facilities, Optimization, Reprints.

Define a design to be any planar set D of known area a , but of unknown shape and location; more generally, a design can be any set in $(R \text{ sub } d)$ of measure a . For example, a design might be one floor of a warehouse, or a sports arena of known seating capacity. Given mild assumptions about the disutility functions, and a slight refinement of the design definition to rule out certain pathologies, the authors present necessary and sufficient conditions for a design to be efficient, and study properties of efficient designs.

500,974

PB86-124831

Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

One-Row Linear Programs.

Final rept.,

C. Witzgall. 1980, 31p

Pub. in Proceedings of International Symposium Extremal Methods and Systems Analysis, Austin, TX., 1977, p384-414 1980.

Keywords: *Linear programming, *Simplex method, Algorithms, Pivot theory.

Motivated by the possibility of improving the efficiency of the dual simplex method, the paper discusses direct solution algorithms for linear programs with upper bounds and generalized upper bounds which apart from bound constraints consist of a single row representing a constraint equation. The close connection between 1-row linear programs with upper bounds and the problem of determining weighted medians is demonstrated. The latter problem is known to be of complexity $O(n)$ where n is the number of variables. A solution algorithm of complexity $O(n \log n) + O(k(n-k))$ is presented for the 1-row k -mix linear program with generalized upper bounds. The algorithm is based on determining the lower boundary of the convex hull of points in the plane.

13.

MECHANICAL, INDUSTRIAL, CIVIL, AND MARINE ENGINEERING

13A. Air Conditioning, Heating, Lighting, and Ventilating

500,975

PATENT-4 501 319

Not available NTIS

Department of the Army, Washington, DC.

Piezoelectric Polymer Heat Exchanger.

Patent,

S. Edelman, and L. D. Ballard. Filed 24 Jan 83, patented 26 Feb 85, 6p PB86-174505, PAT-APPL-6-460 221

Supersedes AD-D010 056.

This Government-owned invention available for U.S. licensing and, possibly, for foreign licensing. Copy of patent available Commissioner of Patents, Washington, DC 20231 \$1.00.

Keywords: *Heat exchangers, *Patents, Heat transfer, Efficiency, Piezoelectric materials, Polymeric films. PAT-CL-165-84.

Disclosed is apparatus for providing for increased heat transfer efficiency of a heat exchanger by separating contiguous fluid conductive channels by means of a flexible sheet fabricated from a piezoelectric polymer. An electrode pattern of predetermined configuration is applied to one or both sides of the piezoelectric sheet and an electrical signal applied thereto in order to set the sheet into a flexural resonance condition whereupon a standing wave pattern is established to not only break up the boundary layer of fluid which adheres to each side of the sheet, but also minimizing the thickness of the laminar sub-layer.

500,976

PB85-167336

CP T05

National Bureau of Standards (NEL), Gaithersburg, MD. Center for Building Technology.

CEL-1: Conservation of Electric Lighting.

Software,

S. Treado. 1 Oct 84, mag tape NBS/DF-85/008

Source tape is in the ASCII character set. This restricts preparation to 9 track, one-half inch tape only. Identify recording mode by specifying density only. Call NTIS Computer Products if you have questions.

Keywords: *Software, *Buildings, *Illuminating, Computerized simulation, Performance, Daylighting, FORTRAN, Windows, CEL 1 computer program, BLAST computer program, Energy analysis, Energy conservation, Computer aided design.

The CEL-1 (Conservation of Electric Lighting) computer program is a design and analysis tool for the design of building lighting systems. It is capable of detailed simulation of lighting system performance, including the effects of daylighting. The interaction between the lighting system and the building heating and cooling systems is accomplished through a custom interface with the BLAST (Building Loads Analysis and System Thermodynamics) building energy analysis program. This tape contains the CEL-1 program Fortran Source files, data files and procedure files, including all updates and changes through 10/1/84. A major addition is the BLAST/CEL-1 interface routine. Software description: The model is written in the FORTRAN programming language for implementation on a CDC 760 computer using the NOS 1.4 Version 528 operating system. Memory requirement is 128 K bytes.

500,977

PB85-177871 PC A02/MF A01
National Bureau of Standards (NEL), Gaithersburg, MD. Building Equipment Div.
Prediction of Performance for a Fire-Tube Boiler with and without Turbulators.
D. Didion, and L. Chern. Aug 84, 25p NBSIR-84/2925
Sponsored by Army Facilities Engineering Support Agency, Fort Belvoir, VA. Technology Support Div.

Keywords: *Fire tube boilers, Performance, Computerized simulation, Efficiency, Turbulators, DEPAB2 computer program.

A series of computer runs were made using DEPAB2 (the boiler simulation computer program). They include the runs for a fire-tube boiler 'as is' (i.e., without turbulators), with wire-coil type turbulators, and with twisted-tape type turbulators, respectively. Output from these runs are used to evaluate the boiler seasonal performance values under the Washington, D.C. weather conditions. Results show that the turbulator increases the boiler seasonal efficiency from 2.87 to 6.08%.

500,978

PB85-177939 PC A06/MF A01
National Bureau of Standards (NEL), Gaithersburg, MD. Building Equipment Div.
HVACSIM(+) Building Systems and Equipment Simulation Program Reference Manual.
D. R. Clark. Jan 85, 111p NBSIR-84/2996
Sponsored by Department of Energy, Washington, DC. Office of Building and Community Systems, and Civil Engineering Lab. (Navy), Port Hueneme, CA.

Keywords: Equipment, Buildings, Control equipment, Air conditioning, Ventilation, Heating, Heating equipment, Computerized simulation, Mathematical models, *Building systems, *HVACSIM+ computer simulation package.

HVACSIM+ is a modular, non-proprietary computer simulation package developed at the National Bureau of Standards, designed to allow detailed simulation of entire building energy systems: the heating, ventilating, and air conditioning (HVAC) system, the equipment control system, the building shell, the physical plant, and the dynamic interactions among these subsystems. The HVACSIM+ package consists of a main simulation program, a library of sub-routines containing mathematical models of building energy system components, and two programs used in preparing a description of the system to be simulated. Models representing the components of a physical plant, such as boilers and chillers, and a model representing a multi-zone building, are under development and will be added to the HVACSIM+ package as they become available.

500,979

PB85-178325 PC A04/MF A01
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Building Technology.
CEL-1 User's Guide Update.
S. J. Treado, C. L. Francisco, and D. B. Holland. Nov 84, 74p NBSIR-84/2974
Sponsored by Civil Engineering Lab. (Navy), Port Hueneme, CA.

Keywords: *Lighting equipment, Illuminance, Irradiance, Daylighting, Systems engineering, CEL-1 computer program, Programming manuals, Energy conservation.

This is a guide to using the CEL-1.1 version of the CEL-1 Lighting Computer Program. CEL-1.1 has the capability of producing hour-by-hour lighting power multipliers for a one-year simulation period. This guide focuses on: (a) the new program routines (b) the interactive capabilities of CEL-1.1 (c) the routines for compiling different types of routines (d) computer terminology and accessing the necessary routines for running CEL-1.1 (e) updates and revisions to the existing CEL-1 manuals.

500,980

PB85-184638 Not available NTIS
Department of Energy, Washington, DC. Office of Solar Heat Technologies.

Performance of Solar Domestic Hot Water Systems at the National Bureau of Standards: Measurements and Predictions.

Final rept.,
A. H. Fanney, and S. A. Klein. 1983, 11p
Sponsored by Department of Energy, Washington, DC. Office of Solar Heat Technologies.
Pub. in Jnl. of Solar Energy Engineering Transactions ASME 105, n3 p311-321 Aug 83.

Keywords: Performance, Measurement, Predictions, Thermodynamic properties, Reprints, *Solar water heating.

This paper includes a detailed description of the hot-water systems, experimental test results, and comparisons with computer predictions using the f-Chart method. The system configurations include an evacuated-tube air system with a cross-flow heat exchanger and two storage tanks, a single-tank direct system, a double-tank direct system, a single-tank indirect system with a wrap-around heat exchanger, a double-tank indirect system with a coil-in-tank heat exchanger, and a thermosyphon system.

500,981

PB85-184679 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Evaluation of Absorber Stagnation Temperature as a Characteristic Performance Parameter of Flat-Plate Solar Collectors.

Final rept.,
A. G. Dawson, W. C. Thomas, and D. Waksman. 1982, 10p
Sponsored by American Society of Mechanical Engineers, New York.
Pub. in Proceedings of the American Society of Mechanical Engineers Winter Annual Meeting 1982, Phoenix, AZ., November 14-19, 1982, Paper No. 82-WA/Sol-5, 10p.

Keywords: *Thermal degradation, Performance tests, Evaluation, Materials, Temperature measurement, Spectral emittance, Thermal conductivity, Absorptance, Transmittance, Meetings, *Solar collectors, *Flat plates, *Stagnation temperature.

An analytical and experimental investigation was undertaken to evaluate an alternate method for measuring the thermal degradation of materials used in flat-plate collectors. This test method is based on measuring the temperature of the absorber under a no-flow condition before and after prolonged exposure. The primary material properties of interest are cover transmittance, solar absorptance and infrared emittance of the absorber, and thermal conductivity of insulation.

500,982

PB85-184703 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Standards for Passive Solar Heating and Cooling Systems.

Final rept.,
R. D. Dijkers, and B. C. Reeder. 1983, 6p
Sponsored by Department of Energy, Washington, DC. Passive and Hybrid Solar Energy Div., and American Society of Mechanical Engineers, New York. Solar Energy Div.
Pub. in Proceedings of the ASME Solar Energy Division Annual Conference (5th), New York, April 18-21, 1983 p103-108.

Keywords: *Standards, Planning, Materials, Components, Tests, Evaluation, *Passive solar cooling systems, *Passive solar heating systems, Assemblies.

The Department of Energy (DOE) Passive Solar Energy Program has been supporting research to develop a technology base for the preparation of uniform test methods, evaluation procedures and other standards for passive solar materials, components, assemblies, and systems. This paper describes the results of a DOE sponsored study to develop an initial planning framework for identifying existing voluntary standards which may be applicable to passive solar technologies as well as needed new standards. The framework described in the study consists of a matrix which can be used by standards writers, builders, manufacturers, engineers and building designers.

500,983

PB85-186955 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Building Equipment Div.

Equation-of-State-Based Thermodynamic Charts for Nonazeotropic Refrigerant Mixtures.

Final rept.,
P. A. Domanski, and D. A. Didion. 1985, 9p
Sponsored by Department of Energy, Washington, DC. and Oak Ridge National Lab., TN.
Pub. in ASHRAE (American Society of Heating, Refrigerating and Air-Conditioning Engineers) Transactions 91, pt. 1, 9p 1985.

Keywords: *Refrigerants, *Thermodynamic properties, Refrigerating machinery, Azeotrope, Mixtures, Charts, Enthalpy, Entropy, Temperature, Pressure, Equations of state, Liquid phases, Vapor phases, Chemical composition, Reprints.

This paper presents thermodynamic charts developed for a nonazeotropic mixture, R13B1/R152a. The developed charts (pressure-enthalpy, temperature-entropy, and enthalpy-composition) offer important insight for understanding vapor compression cycles for different compositions. An equation of state capable of describing both the liquid and vapor phases, property algorithms and iteration schemes used in determination of the nonazeotropic mixture thermodynamic properties have been explained.

500,984

PB85-187441 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Temperature Calibration for Solar Heating and Cooling System Evaluation.

Final rept.,
J. F. Schooley. 1978, 5p
Pub. in Conference on Performance Monitoring Techniques for Evaluation of Solar Heating and Cooling Systems, Washington, DC, April 3-4, 1978, p307-311.

Keywords: *Calibrating, *Temperature measuring instruments, *Solar heating, Monitors, Performance evaluation, *Solar cooling systems.

Problems associated with the calibration of temperature instrumentation for performance monitoring of solar systems are briefly discussed. A short outline is presented of thermometer calibration services and associated programs available at the National Bureau of Standards.

500,985

PB85-191963 PC A05/MF A01
National Bureau of Standards (NEL), Gaithersburg, MD. Building Equipment Div.
Field Performance of Three Residential Heat Pumps in the Cooling Mode.
W. H. Parken, D. A. Didion, P. H. Wojciechowski, and L. Chern. Mar 85, 82p NBSIR-85/3107

Keywords: *Heat pumps, Residential buildings, Thermostats, Cooling systems, Air conditioning, Field tests, Performance evaluation, Tests, Efficiency, Data acquisition, Energy conservation.

Field data was acquired for three residential heat pumps and the part load performance factor and seasonal cooling energy efficiency ratio were evaluated. Laboratory tests were conducted on a unit identical to one of the field-tested heat pumps and performance results compared. Thermostat data was also acquired and a semi-empirical model developed.

500,986

PB85-195956 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Design and Analysis of Passive Solar Heating Solutions for Neighborhood Commercial Strip Settings.

Final rept.,
K. Ruberg. 1979, 5p
Pub. in Proceedings of the National Passive Solar Conference (4th), Kansas City, MO., October 3-5, 1979 p576-580.

Keywords: *Commercial buildings, Design, Thermal analysis, Performance, Urban areas, *Passive solar heating systems, Energy conservation, Energy consumption.

As part of an NBS study on urban solar applications, two passive solar heating methods and preliminary thermal performance data are described for a prototypical neighborhood commercial strip.

500,987

PB85-197556 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.

Field 13—MECHANICAL, INDUSTRIAL, CIVIL, AND MARINE ENGINEERING

Group 13A—Air Conditioning, Heating, Lighting, and Ventilating

Flow Rate Calibration for Solar Heating and Cooling System Evaluation.

Final rept.,
G. E. Mattingly. 1978, 7p
Pub. in Proceedings of Conference on Performance Monitoring Techniques for Evaluation of Solar Heating and Cooling Systems, Washington, DC., April 3-4, 1978, p299-305.

Keywords: *Calibrating, *Flow rate, Flow measurement, Flowmeters, Performance evaluation, Solar heating, *Solar collectors, Solar cooling systems.

A description is given of the flow metering calibration facilities at the National Bureau of Standards that pertain to solar collectors and the instrumentation required to evaluate their performance. Alternative methods are also briefly described for obtaining the quantified assurance that the pertinent flow measurements are as good as they are quoted to be. Flow metering problem areas are also discussed with suggestions for preventative or remedial action.

500,988

PB85-197663

Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

Rating Procedure for Solar Domestic Water Heating Systems.

Final rept.,
S. A. Klein, and A. H. Fanney. 1983, 10p
Sponsored by Department of Energy, Washington, DC. Office of Solar Heat Technologies.
Pub. in Jnl. of Solar Energy Engineering 105, n4 p430-439 Nov 83.

Keywords: Ratings, Standards, Tests, Reprints, *Solar water heating, Residential sector.

A rating procedure for solar domestic hot water systems is described which combines the advantages of short-term system tests and correlations of long-term thermal performance. The testing procedure consists of two indoor tests which are in accordance with ASHRAE Standard 95-1981 except for one additional measurement needed only for systems employing a heat exchanger between the collector fluid and the potable water. The test results are plotted in a manner in which they can be used to estimate the long-term performance of the solar water heating system for any location where site-specific monthly-average meteorological data are available. The annual solar fraction obtained in this manner provides the recommended rating indicator. The validity of this rating procedure is first demonstrated by simulations. Further support is provided by experiments conducted at the National Bureau of Standards.

500,989

PB85-198927

PC A04/MF A01

National Bureau of Standards (NEL), Gaithersburg, MD. Center for Building Technology.

Laboratory Tests of a Gas Fueled Modulating Type Hot Water Boiler.

E. R. Kweiller. Apr 85, 59p NBSIR-85/3142
Sponsored by Department of Energy, Washington, DC.

Keywords: *Boilers, *Hot water heating, Space heaters, Simulation, Fuel consumption, Gas furnaces, Efficiency, Tests, Heat transfer, *Gas fired.

The objective of this study was to set up a modulating controlled hot water boiler in the laboratory and to simulate a variety of conditions that were cited by manufacturers of boilers as influencing and being distinct operating parameters for boilers. A further objective of these tests was to compare these responses of the fuel input rate with the mode of operation which was previously described for modulating controlled space heaters and furnaces. The variation of controlled fuel rate to the burner via the fuel modulating valve was measured under several controlled conditions. Effects of heating load, burner cycling rate and zone control, were investigated. The response of gas pressure modulation to the burner of a hot water boiler heating system was studied in several series of tests in the laboratory. A boiler load simulator was set up and used for these tests to control the heating load (heat transfer rate at the radiators) and to simulate a variety of operating conditions that would be expected to exist with a boiler installed in the home. The effects of heat transfer rate and boiler water operating temperature on the modulated gas pressure are presented as a series of data in charts showing controlled gas pressure versus time.

500,990

PB85-201804

Not available NTIS

National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div.

Recent Developments in Self-Contained Cryocoolers for SQUIDS and Other Low-Power Cryoelectronic Devices.

Final rept.,
J. E. Zimmerman. 1984, 7p
Pub. in Proceedings of Int. Cryogenic Engineering Conference (10th), Helsinki, Finland, July 31-August 3, 1984, p13-19.

Keywords: *Refrigerators, Cryogenics, *Cryocoolers, SQUID devices.

The particular requirements of refrigeration for very low power cryoelectronic devices have been addressed only during the last few years. A number of laboratory prototypes are now near realization, and commercial systems may be available soon. These include Stirling and Gifford-McMahon machines and a four-stage Joule-Thomson machine, or a combination of one of the former with a final Joule-Thomson stage to achieve 4K, and small liquid-helium cryostats with integral intermittent reliquefying capability. The most difficult technical problem outstanding is to design reliable, non-contaminating, miniature compressors for these machines.

500,991

PB85-203537

Not available NTIS

National Bureau of Standards (NEL), Gaithersburg, MD. Fire Safety Technology Div.

Analysis of the Forced Ventilation in Container-ship Holds.

Final rept.,
H. R. Baum, and J. A. Rockett. 1984, 34p
Sponsored by Coast Guard, Washington, DC.
Pub. in Jnl. of Fluid Mechanics 142, p309-342 1984.

Keywords: *Ventilation, *Cargo ships, Mass transfer, Fluid flow, Computer programs, Hazardous materials, Fires, Reprints, Fire models.

An analysis of the fluid flow and mass transfer induced by ventilation systems in container-ship holds was carried out. The analysis consists of a detailed calculation of the forced motion through an interconnected set of narrow, stably stratified vertical air passages which represent an idealized container-ship hold. The results of the calculation are then used in a study of the concentration boundary layers formed by the pickup of spill material assumed to lie at the bottoms of the air passages. The results are incorporated in a computer program which is described in detail. A variety of computed results are presented, together with a listing of the program.

500,992

PB85-205151

Not available NTIS

National Bureau of Standards (NEL), Gaithersburg, MD. Building Equipment Div.

Experimental and Analytical Evaluation of Collector Storage Walls in Passive Solar Applications.

Final rept.,
M. E. McCabe, C. E. Hancock, and J. Seem. Oct 84, 5p
Sponsored by Department of Energy, Washington, DC. Passive and Hybrid Solar Energy Div.
Pub. in Proceedings of the Passive and Hybrid Solar Energy Update, Washington, DC., September 5-7, 1984, p38-42.

Keywords: *Walls, Concrete blocks, Masonry, Test facilities, Heat measurement, Calorimeters, Thermal measurements, Heat transfer, *Passive solar heating systems, *Energy storage, *Solar collectors.

Studies of the thermal performance of passive solar buildings have indicated a need for precise measurement of solar and thermal energy transfer in modular passive/hybrid solar components under conditions of actual use. A calorimetric test facility designed for performance testing of passive solar components provided test data for several passive solar components during 1983/1984 winter test season. A description of the test facility is presented along with a summary description of four collector-storage wall (CSW) components tested. One of these components, a CSW consisting of a double-glazed window and non-vented concrete masonry block wall with a radiatively selective foil on the outer surfaces was characterized using transfer function techniques. The study suggests that the transfer function analysis technique is well suited for correlating dynamic heat transfer measurements to the environmental variables of solar irradiance and ambient temperature.

500,993

PB85-205250

Not available NTIS

National Bureau of Standards (NEL), Gaithersburg, MD. Building Equipment Div.

Sensor Errors.

Final rept.,
J. Y. Kao. Jan 85, 5p
Pub. in ASHRAE (American Society of Heating, Refrigerating and Air-Conditioning Engineers) Jnl. 27, n1 p100-104 Jan 85.

Keywords: *Sensors, *Air circulation, Errors, Automatic control equipment, Computerized simulation, Buildings, Reprints, *Energy consumption, Building systems.

The paper examines the energy effect of sensing errors of an air handling system. The energy waste caused by errors of various automatic control sensors in a variable air volume system are simulated with a computer program and the results are presented and discussed. Some sensing errors cause substantial energy waste. The paper also describes the causes of sensing errors frequently seen in an air handling system - from building design and installation to building operation. Recommendations for minimizing these errors are given.

500,994

PB85-205961

Not available NTIS

National Bureau of Standards (NEL), Gaithersburg, MD.

Test Methods and Procedures for Passive Solar Components and Materials.

Final rept.,
R. D. Dikkers. 1982, 3p
Sponsored by Department of Energy, Washington, DC. Passive and Hybrid Solar Energy Div.
Pub. in Proceedings of U.S. Department of Energy Passive and Hybrid Solar Energy Program Update, Washington, DC., August 9-12, 1981, Conf-810832, p3.41-3.43 1982.

Keywords: *Solar heating, *Tests, Standards, Space heatings, Buildings, *Passive solar heating systems.

The National Bureau of Standards (NBS) is assisting the Department of Energy and other organizations in the development of test methods and evaluation procedures for passive solar systems, components and materials. This paper describes three pertinent NBS projects: (1) the development of a general plan to identify needed test methods and other standards; (2) the identification of health and safety issues and related building code provisions; and (3) the development of test methods to measure the thermal performance of passive/hybrid solar components.

500,995

PB85-207173

Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

Thermal Performance Comparisons for a Solar Hot Water System.

Final rept.,
R. A. Fisher, and H. A. Fanney. 1983, 5p
Sponsored by Department of Energy, Washington, DC. Pub. in ASHRAE (American Society of Heating, Refrigeration and Air-Conditioning Engineers) Jnl. 25, n8 p27-31 1983.

Keywords: Hot water heating, Thermal efficiency, Performance, Reprints, *Solar water heaters.

The performance of two identical solar domestic hot water (SDHW) heaters subjected to various load profiles is compared. Three hourly load profiles having the same total daily load and two variations in total daily load are considered. Comparisons are made based on measured performance for two double-tank direct solar hot water systems located at the National Bureau of Standards Solar Test Facility. The experimental investigation reveals that load profiles have a small effect on the thermal performance of a typical SDHW system.

500,996

PB85-224459

PC A05/MF A01

National Bureau of Standards (NEL), Gaithersburg, MD. Center for Building Technology.

Laboratory Design and Test Procedures for Quantitative Evaluation of Infrared Sensors to Assess Thermal Anomalies,
Y. M. Chang, and R. A. Grot. Jun 85, 86p NBSIR-85/3131

Sponsored by Department of Energy, Washington, DC. Prepared in cooperation with DCS Corp., Alexandria, VA.

Keywords: *Infrared thermal detectors, Evaluation, Tests, Calibrating, Temperature, Buildings, Variability, Display devices, Infrared radiation, Heat loss, *Infrared thermography, Modulation transfer functions.

The report presents the description of the laboratory apparatus and preliminary results of the quantitative evaluation of three high-resolution and two low-resolution infrared imaging systems. These systems which are commonly used for building diagnostics are tested under various background temperatures (from -20C to 25C) for their minimum resolvable temperature differences (MRTD) at spatial frequencies from 0.03 to 0.25 cycles per milliradian. The calibration curves of absolute and differential temperature measurements are obtained for three systems. The signal transfer function and line spread function at ambient temperature of another three systems are also measured. Comparisons of the dependence of the MRTD on background temperatures from the measured data with the predicted values given in ASHRAE Standards 101-83 are also included. The dependence of background temperatures for absolute temperature measurements are presented, as well as comparison of measured data and data given by the manufacturer. Horizontal on-axis magnification factors of the geometric transfer function of two systems are also established to calibrate the horizontal axis for the measured line spread function to obtain the modulation transfer function. The variation of the uniformity for horizontal display of these two sensors are also observed. Included are detailed descriptions of laboratory design, equipment setup, and evaluation procedures of each test.

500,997

PB85-233369 PC A13/MF A01
National Bureau of Standards, Boulder, CO.

Proceedings of the Cryocooler Conference (3rd) Held at Boulder, Colorado on September 17-18, 1984,

R. Radebaugh, B. Louie, and S. McCarthy. May 85, 283p NBS/SP-698

Also available from Supt. of Docs as SN003-003-02662-0. Library of Congress catalog card no. 85-600544. Sponsored by National Aeronautics and Space Administration, Greenbelt, MD. Goddard Space Flight Center, Naval Research Lab., Washington, DC. and Office of Naval Research, Arlington, VA.

Keywords: *Refrigerators, *Meetings, Superconductors, Infrared detectors, Refrigerating, Cryopumping, Cryogenics, Helium, *Cryocoolers, *Cryogenic refrigerators, Magnetic refrigerators.

The document contains the proceedings of the Third Cryocooler Conference, held at the National Bureau of Standards, Boulder, CO, on Sept. 17-18, 1984. About 140 people from 10 countries attended the conference and represented industry, government, and academia. A total of 26 papers were presented orally at the conference and all appear in written form in the document. The emphasis in the conference was on small cryocoolers in the temperature range of 4-80K. Mechanical and non-mechanical types were discussed in the various papers. Applications of the small cryocoolers include the cooling of infrared detectors, cryopumps, small superconducting devices and magnets, and electronic devices.

500,998

PB85-242204 PC A07/MF A01
National Bureau of Standards (NEL), Boulder, CO. Chemical Engineering Science Div.

Round Robins on the Apparent Thermal Conductivity of Low-Density Glass Fiber Insulations Using Guarded Hot Plate and Heat Flow Meter Apparatus,
J. G. Hust, and C. M. Pelanne. May 85, 133p NBSIR-85/3026

Sponsored by Oak Ridge National Lab., TN., American Society for Testing and Materials, Philadelphia, PA., and Mineral Insulation Mfrs. Association, Summit, NJ. Prepared in cooperation with Thermal Insulation, Littleton, CO.

Keywords: *Thermal insulation, *Glass fibers, *Thermal conductivity, Measurement, Heat transmission, Thickness.

The report presents the results and the data analysis pertaining to the results for three round robins on the thermal performance of guarded hot plates and heat flow meters when measuring the thermal resistance properties of low density glass fibrous thermal insulations. The three round robins were carried out under the sponsorship of the American Society for Testing and Materials (ASTM) Subcommittee C-16.30 on Thermal Measurements and the Mineral Insulation Manufacturers Association (MIMA). The test results are compared to a reference equation and to each other to illustrate intralaboratory and interlaboratory reproducibility as well as the dependencies on temperature, density, plate emittance, specimen thickness, and fiber diameter.

500,999

PB86-103462 PC A03/MF A01
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Building Technology.

Ventilation Effectiveness in Mechanically Ventilated Office Buildings,

A. K. Persily. Aug 85, 40p NBSIR-85/3208
Sponsored by Department of Energy, Washington, DC. Office of Building and Community Systems.

Keywords: *Ventilation, *Office buildings, Efficiency, Effectiveness, Measurement, Measuring instruments, Air flow, *Air quality, Air infiltration.

The paper examines several definitions of ventilation effectiveness and associated tracer gas measurement techniques. Techniques for making ventilation effectiveness measurements in mechanically ventilated office buildings are discussed with reference to building and mechanical equipment design and tracer gas instrumentation. Specific strategies are proposed for measuring ventilation effectiveness on different scales ranging from individual rooms to whole buildings.

501,000

PB86-108198 PC A05/MF A01
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Building Technology.

Review of Energy Use Factors for Selected Household Appliances,

J. Greenberg, B. Reeder, and S. Silberstein. 19 Aug 85, 87p NBSIR-85/3220

Contract DE-AI01-76PR06010
Sponsored by Department of Energy, Washington, DC. Office of Buildings Energy R and D.

Keywords: *Buildings, *Electric appliances, Standardization, Tests, Furnaces, Water heaters, *Energy efficiency standards, Energy consumption, Consumption rate, Energy efficiency.

The Energy Policy and Conservation Act (EPCA) as amended by the National Energy Conservation Policy Act (NECPA) requires the development of test procedures, labeling rules, and energy efficiency standards for consumer appliances. The purpose of this report is to re-evaluate selective parametric values through analysis of current data, and provide comment and recommendations. The parameters reviewed are: For water heaters - inlet water temperature, outlet water temperature, ambient air temperature, and hot water usage; for furnaces - outdoor design temperature and average annual heating hours; for room and central air conditioners - yearly hours of use. Each parameter reviewed is documented in an independent section in this report and indicates the current value, the historical basis for the current value, the approach used to review and update the value, the results and conclusions, and recommendations. The recommendations generally propose a new value for the parameter studied based upon the information analyzed.

501,001

PB86-111846 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Building Physics Div.

Boiling Tests of Thermal Insulation in Conduit-Type Underground Heat Distribution Systems.

Final rept.,
T. Kusuda, and W. M. Ellis. 1983, 17p
Pub. in Proceedings of Thermal Insulation, Materials, and Systems for Energy Conservation in the 80's, Clearwater Beach, FL., December 8-11, 1981, ASTM STP 789, p802-818 1983.

Keywords: *Heat distributing units, Boiling, Tests, Thermal insulation, Piping systems, Test equipment, Specifications, Energy conservation.

Thermal insulation in a conduit-type underground heat distribution system is expected to withstand severe

boiling, which could occur in the case of conduit failure under high ground-water table. The U. S. Government specifies boiling-test criteria for the approval of commercial underground systems. The paper describes the test apparatus and procedure of Tri-Services and Federal Agencies' Specifications to evaluate thermal performance of various insulations after they are subjected to prolonged boiling conditions.

501,002

PB86-113958 PC A04/MF A01
National Bureau of Standards (NEL), Gaithersburg, MD. Building Equipment Div.

Laboratory Study of Gas-Fueled Condensing Furnaces,

E. R. Kweller, and R. A. Wise. Jul 85, 51p NBSIR-85/3225

Sponsored by Department of Energy, Washington, DC. Office of Buildings Energy R and D.

Keywords: *Gas furnaces, *Steam condensers, Performance evaluation, Experimental design, Temperature measurement, Humidity, Design criteria.

The objective of the study was to determine if the direct measurement method of condensate collection that was developed during prior testing of a condensing boiler would be adequate for direct measurement of the condensate from gas fueled forced warm air condensing furnaces. Results of these tests were for purposes of supporting a test procedure proposed by the Department of Energy and responding to questions raised in comments to the proposed procedures. Another objective of these tests was to quantify the effects of varying test room ambient temperatures and relative humidity in the rate of condensate collected with condensing furnaces.

501,003

PB86-122868 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Building Physics Div.

Method of Testing Passive Storage Walls to Determine Thermal Performance.

Final rept.,
M. McCabe, M. McKinstry, and P. Wormser. 1979, 3p
Sponsored by Department of Energy, Washington, DC. Office of Conservation and Solar Energy.
Pub. in Proceedings of National Passive Solar Conference (4th), Kansas City, MO., October 3-5, 1979, p736-738.

Keywords: *Thermal analysis, Performance tests, Finite difference theory, Walls, Buildings, Heat storage, Computerized simulation, *Trombe walls, *Passive solar heating systems.

A conceptual thermal performance test for passive solar storage walls is described. The test procedure applied to a Trombe-Wall is evaluated by computer simulation, using a finite-difference thermal model. A simple calculation procedure for a building using the Trombe-Wall pseudo test results is described and the thermal performance estimates are shown to compare reasonably well with the results predicted by the detailed computer model simulation.

501,004

PB86-122926 Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Chemical Engineering Science Div.

Stirling Cycle and Cryogenic Refrigerators.

Final rept.,
B. Louie, and R. Radebaugh. 1984, 6p
Pub. in Proceedings of IECEC '84 Advanced Energy Systems-Their Role in Our Future (19th), San Francisco, CA., August 19-24, 1984, p2086-2091.

Keywords: *Stirling cycle, Thermodynamic cycles, Reliability, *Cryogenic refrigerators, *Cryocoolers.

The paper reviews the principles and techniques used in cryogenic refrigeration, with particular emphasis on small cryocoolers. Several thermodynamic cycles used in cryocoolers are discussed, as are the design requirements, applications, and current areas of research. The important features of the Stirling cycle used as a prime mover or refrigerator are compared.

501,005

PB86-124930 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Operations Research Div.

Field 13—MECHANICAL, INDUSTRIAL, CIVIL, AND MARINE ENGINEERING

Group 13A—Air Conditioning, Heating, Lighting, and Ventilating

Acoustical Benefits and Costs of Passive Solar Energy Design.

Final rept.,
R. T. Ruegg, and W. F. Danner. 1982, 6p
Pub. in Proceedings of National Passive Solar Conference (7th), Knoxville, TN., August 30, 1982, p589-594.

Keywords: *Acoustics, *Benefit cost analysis, Buildings, Heating, *Passive solar heating systems.

The purpose of this paper is to develop a framework for the maximization of joint thermal and acoustical net benefits from passive solar design. The paper first identifies the circumstances in which acoustical benefits and costs tend to occur in conjunction with passive solar design, and outlines some simple steps for enhancing beneficial acoustical effects and reducing adverse effects. It then incorporates acoustical effects of passive solar design into a life-cycle benefit-cost framework.

501,006
PB86-129772 PC A04/MF A01

National Bureau of Standards (NEL), Gaithersburg, MD. Center for Building Technology.

Validation Tests of the Thermal Analysis Research Program.

G. N. Walton, and K. Cavanaugh. Sep 85, 52p
NBSIR-85/3211

Keywords: *Buildings, *Thermal analysis, Tests, Research projects, Computerized simulation, Energy analysis.

In the study analytical and empirical tests were performed using the Thermal Analysis Research Program (TARP). TARP was found to be very accurate relative to the analytical tests (calculations for simplified conditions) which covered steady and transient conduction, internal radiant interchange, latent loads, and clear sky solar gains. Six one-room buildings with different wall constructions provided data for the empirical tests.

501,007
PB86-130614 PC A10/MF A01

National Bureau of Standards (NEL), Gaithersburg, MD. Building Equipment Div.

HVACSIM+ Building Systems and Equipment Simulation Program - Users Guide.

D. R. Clark, and W. B. May. Sep 85, 203p NBSIR-85/3243

See also PB85-177939. Sponsored by Department of Energy, Washington, DC. Office of Building and Community Systems, and Civil Engineering Lab. (Navy), Port Hueneme, CA.

Keywords: *Environmental engineering, *Computerized simulation, Buildings, *Building systems, *HVAC-SIM (+) computer program.

HVACSIM+ is a modular, non-proprietary computer simulation package developed at the National Bureau of Standards. The package consists of a general-purpose modular simulation program called MODSIM, a library of component models specific to building systems, and a simulation editor called HVACGEN. The latter is used to facilitate the creation and modification of simulation descriptions. HVACSIM+ is designed to allow detailed simulation of entire building systems or portions of such systems. This includes the heating, ventilating, and air conditioning (HVAC) system, the equipment control system, the conditioned zones within a building, the building shell, and the dynamic interactions among these subsystems. This document describes the procedures for installing HVACSIM+ on a particular computer, for setting up a simulation description using HVACGEN, and for running a simulation using MODSIM.

501,008
PB86-136801 Not available NTIS

National Bureau of Standards (NEL), Gaithersburg, MD. Center for Building Technology.

Mathematical Model of an Air-to-Air Heat Pump Equipped with a Capillary Tube.

Final rept.,
P. Domanski, and D. Didion. 1984, 7p
Pub. in International Jnl. of Refrigeration 7, n4 p249-255 Jul 84.

Keywords: Heat pumps, Capillary tubes, Computerized simulation, Reprints, *Air source heat pumps.

The paper describes in general a computer model for simulation of steady-state performance of a split, residential, air-to-air heat pump. Organization of the model

is discussed and approach to modelling of main heat pump components is explained. The modelling effort emphasis was on the local phenomena to be described by fundamental thermodynamic, heat transfer and fluid mechanic relationships. The model has been verified in a wide range of operating conditions from high temperature cooling to low temperature heating.

501,009
PB86-137981 Not available NTIS

National Bureau of Standards (NEL), Gaithersburg, MD. Building Physics Div.

Heat Loss Due to Thermal Bridges in Buildings.

Final rept.,
J. B. Fang, R. A. Grot, K. W. Childs, and G. E. Courville. 1984, 9p
Sponsored by Department of Energy, Washington, DC. Pub. in Proceedings of the Society of Photo-Optical Instrumentation Engineers International Conference on Thermal Infrared Sensing for Diagnostics and Control (Thermosense 6), Oak Brook, IL., October 2-5, 1983, v446 p34-42 1984.

Keywords: *Heat loss, Office buildings, Heat transmission, *Heat flow, Infrared thermography.

Building envelopes often contain numerous highly conductive heat flow paths, called thermal bridges, which are major sources of heat loss and areas of deterioration of building materials due to moisture condensation. Some examples of thermal bridges occurring in office buildings are presented. Infrared thermography was used to identify the locations and magnitudes of thermally defective areas resulting from inadequate construction, design, or substandard workmanship in existing buildings.

501,010
PB86-137999 Not available NTIS

National Bureau of Standards (NEL), Gaithersburg, MD. Building Equipment Div.

Experimental-Technique for Testing Thermosyphon Solar Hot Water Systems.

Final rept.,
A. H. Fanney. 1984, 8p
Sponsored by Department of Energy, Washington, DC. Pub. in Jnl. of Solar Energy Engineering-Transactions of the ASME (American Society of Mechanical Engineers) 106, 4 p457-464 1984.

Keywords: *Performance tests, Evaluation, Ratings, Reprints, *Solar water heating, *Thermosyphon effect, Solar collectors.

An experimental technique for testing thermosyphon solar hot water systems is described which allows testing of the system indoors under nonirradiated conditions. The technique described is applicable to thermosyphon systems which utilize flat-plate solar collectors. Energy normally absorbed by the irradiated solar collectors is supplied by electric strip heaters attached to the back side of the absorber plates. Analytical expressions are developed which allow the power input to the strip heaters to be calculated for various environmental conditions. A description of the experimental apparatus and test procedure is given. Results are presented which show that the performance of a thermosyphon system tested indoors using the electric strip heater technique closely duplicates system performance under outdoor irradiated conditions.

501,011
PB86-138005 Not available NTIS

National Bureau of Standards (NEL), Gaithersburg, MD. Building Equipment Div.

Review of Solar Domestic Hot Water System Test and Rating Procedures.

Final rept.,
A. H. Fanney. 1983, 9p
Sponsored by Department of Energy, Washington, DC. Office of Solar Heat Technologies.
Pub. in Proceedings of Annual Conference of American Society of Mechanical Engineers Solar Energy Division (5th) -- Solar Engineering 1983, Orlando, FL., April 18-21, 1983, p169-177.

Keywords: *Tests, *Ratings, Standards, Hot water heating, *Solar water heating, Solar water heaters.

The paper reviews various test methods and rating standards which are currently (October 1982) being considered for solar hot water systems. Test and rating standards proposed in America, Australia, Canada, and South Africa are discussed.

501,012
PB86-138211 Not available NTIS

National Bureau of Standards (NEL), Gaithersburg, MD. Building Physics Div.

Assessment of the Application of Thermography for the Quality Control of Weatherization Retrofits.

Final rept.,
R. A. Grot. 1980, 16p
Sponsored by Department of Energy, Washington, DC. Pub. in Proceedings of National Conference on Thermal Infrared Sensing Technology for Energy Conservation Programs (2nd), Thermosense 2, Albuquerque, New Mexico, November 7-9, 1979, p193-208 1980.

Keywords: *Residential buildings, Thermal insulation, Quality control, *Weatherization.

Approximately 65 single-family low-income homes in eight cities (Portland, Maine; Minneapolis/St. Paul, Minnesota; Fargo, North Dakota; Tacoma, Washington; St. Louis, Missouri; Washington, D.C.; Atlanta, Georgia; and Charleston, South Carolina) were retrofitted using such weatherization techniques as caulking and weatherstripping, adding attic insulation, installing storm windows and doors, insulating basements and crawl spaces, and insulating exterior walls with either ureaformaldehyde (UF) foam or blown-in cellulosic insulation. Thermographic surveys of these dwellings were performed after the weatherization work was completed in order to assess the quality of workmanship and to determine the percentage of wall not insulated by the contractors, and other defects which still existed in the dwelling.

501,013
PB86-155488 PC A04/MF A01

National Bureau of Standards (NEL), Gaithersburg, MD. Chemical Process Metrology Div.

Report on the NBS-DOE (National Bureau of Standards-Department of Energy) May 1984 Workshop on Thermal Metering.

Final rept.,
G. E. Mattingly. Nov 85, 59p NBSIR-85/3242
Sponsored by Department of Energy, Washington, DC. Office of Conservation.

Keywords: *District heating, *Thermal measurement, Standards, Two-phase flow, *District cooling, Energy conservation.

A workshop on thermal metering (i.e., the flow of steam or of hot or chilled water) was convened in Gaithersburg, MD, May 21-22, 1984 to discuss and prioritize flow rate measurement problems and research programs which could lead to improved energy conservation through the development, acceptance, and use of district heating and cooling systems. The workshop brought together 60 attendees whose expertise spanned a broad range of interests. Included were flowmeter manufacturers, meter users, standards personnel, academicians, and consultants. Attendees listed current problem areas and measurement needs in thermal metering, discussed appropriate responses to these needs, and prioritized these according to their perceived potential for impacting thermal metering practices. Leading this list are: 'paper' standards with special emphasis on 'meter installation requirements', research on two-phase flow and its measurement, two-phase flow technology transfer and information dissemination.

501,014
PB86-163821 PC A07/MF A01

National Bureau of Standards (NEL), Gaithersburg, MD. Building Equipment Div.

Building Emulation Computer Program for Testing of Energy Management and Control System Algorithms.

W. B. May, and C. Park. Dec 85, 133p NBSIR-85/3291
Sponsored by Civil Engineering Lab. (Navy), Port Hueneme, CA., and Department of Energy, Washington, DC. Office of Building and Community Systems.

Keywords: *Buildings, *Computerized simulation, Computer programs, Heating, Ventilation, Air conditioning, Algorithms, Control equipment, *Energy management.

A building emulator can be used to test energy management and control systems (EMCS). The emulator uses a computer program to simulate the responses of a building including the equipment, building space, and building envelope to EMCS commands. Building model software for the emulator has been developed at the National Bureau of Standards (NBS) in an effort to assist the United States Naval Civil Engineering Labo-

ratory (NCEL), which is developing a sophisticated building emulator. The concept of the building emulator and the building emulator computer program are described in this report. The program includes the weather, the air handling unit, the zone, and the comfort model. In addition, the energy compilation routine is also included. The models presented here are simplified models. With these abridged models, a single zone building with exterior walls and a single deck air handling unit are simulated. A complete FORTRAN source code of the building emulator computer program is appended.

13B. Civil Engineering

501,015

PB85-212306

PC A02/MF A01

National Bureau of Standards (NEL), Gaithersburg, MD. Building Physics Div.

Indoor Air Quality Modeling Workshop Report,

P. E. McNall, May 85, 16p NBSIR-85/3150

Sponsored by Environmental Monitoring Systems Lab., Research Triangle Park, NC.

Keywords: *Air pollution control, *Mathematical models, *Regulations, Absorption, Air circulation, National government, *Indoor air pollution, *Air quality.

Comprehensive modeling of emission, absorption, movement, and controls of indoor air contaminants is essential for developing national policy for IAQ assessment and controls. This report describes several topics discussed in a workshop on indoor air quality, which was held on February 11, 1985 at the National Bureau of Standards. Researchers on IAQ modeling were invited to state their current activities, identify future research needs and recommend specific parameters and contaminants to be included in the IAQ models. The input thus obtained in this workshop will be incorporated in an advanced simulation model for IAQ, to be developed by NBS under a contract with EPA.

501,016

PB85-246502

PC A07/MF A01

National Bureau of Standards (NEL), Gaithersburg, MD. Center for Applied Mathematics.

Paratransit Advanced Routing and Scheduling System Documentation: Routing and Scheduling Dial-A-Ride Subsystem,

H. K. Hung, W. G. Hall, and R. E. Chapman. Jul 85, 146p NBSIR-85/3178

Sponsored by Urban Mass Transportation Administration, Washington, DC.

Keywords: Routing, Scheduling, Algorithms, Fortran, *Paratransit, *Dial a ride systems, Computer software, Advanced Routing and Scheduling System.

The Advanced Routing and Scheduling System (ARSS) is a software system designed to route and schedule patrons in a dial-a-ride environment. The system consists of three subsystems: CONENV, a pre-processor which constructs physical and policy environments; RSDAR, which routes and schedules patrons; and GREPOR, which generates hard copy of all necessary reports. This report provides a description of RSDAR. The RSDAR is a heuristic algorithm. It assigns patrons to form subgroups in time intervals, and these subgroups are linked to become a tour. Patrons are chosen to be included in a subgroup on the basis of the best remaining time of the base trip. Subgroups are selected to be included in a tour on the basis of the best productivity measure. The model is written in FORTRAN and complies with the American National Standards Institute X3.9-1978 standard for that language.

501,017

PB86-112380

Not available NTIS

National Bureau of Standards (NEL), Gaithersburg, MD. Statistical Engineering Div.

Statistical Aspects of Designs for Studying Sources of Contamination.

Final rept.,

W. Liggett. 1985, 19p

Pub. in American Society for Testing and Materials, Special Technical Publication 867, p22-40 1985.

Keywords: *Statistical analysis, *Environmental surveys, *Ground water, *Waste management, *Solid

waste disposal, Sources, Design criteria, Sampling, Sites, Experimental design, Water pollution, Assessments, Reprints, *Pollution monitoring, *Waste processing plants.

A design for studying sources of environmental contamination must start with a basis for distinguishing the contamination of interest from the background. As part of this basis, the design should provide a method for assessing the sampling and measurement error. Because of problems with reports of none detected, the design should also include a plan for analyzing intermediate laboratory results in addition to the reported values. This paper discusses these aspects of design in the context of monitoring the groundwater around a waste management facility. A design appropriate for spatially and temporally varying backgrounds is proposed and illustrated with monitoring results from Alabama and Florida. To assess the sampling error, the proposed design specifies resampling each well after a period of a few days. Experiments to check this procedure are suggested. The proposed design incorporates and supplements the Environmental Protection Agency laboratory method for total organic halide. In addition, this paper illustrates some difficult design problems that involve nonnormality and nonlinear measurement methods.

501,018

PB86-133527

Not available NTIS

National Bureau of Standards (NEL), Gaithersburg, MD. Operations Research Div.

Evaluating the Risks of Solid Waste Management Programs: A Suggested Approach.

Final rept.,

R. E. Chapman, and H. Yakowitz. 1984, 18p

Pub. in Resour. Conserv. 11, n2 p77-94 Nov 84.

Keywords: *Waste management, *Mathematical models, Substitutes, Risks, Monte Carlo method, Cost analysis, Capitalized costs, Assessments, Reprints, *Solid wastes, *Resource recovery facilities.

The focus of the paper is on how the Resource Recovery Planning Model (RRPLAN) can be used to evaluate the risks associated with alternative solid waste management programs. The paper first discusses how RRPLAN uses a detailed cost accounting framework to weigh the consequences of decisions affecting siting, routing, marketing and financing. A case study of the tri-county area surrounding Jackson, Mississippi, where two waste-to-energy facilities are compared to an all landfill option, is then introduced. The case study shows how a coordinated sensitivity analysis can be used to develop a cost estimating relationship between the discounted cost per ton of processing at a waste-to-energy facility and three explanatory variables: (1) the capital cost of the facility; (2) the volume of waste processed; and (3) revenues from the sale of recoverables and any associated tipping fees. A Monte Carlo experiment is then performed to show how variations about the expected values for the three explanatory variables affect the risk of the program. The probability that the discounted cost per ton of the waste-to-energy facility exceeds that of the all landfill option is used as a risk assessment mechanism.

501,019

PB86-140514

PC A07/MF A01

National Bureau of Standards (NEL), Gaithersburg, MD. Building Physics Div.

Validation of Models for Predicting Formaldehyde Concentrations in Residences Due to Pressed Wood Products. Phase 1,

R. A. Grot, S. Silberstein, and K. Ishiguro. Sep 85,

148p NBSIR-85/3255

Sponsored by Consumer Product Safety Commission, Washington, DC.

Keywords: *Formaldehyde, *Mathematical models, *Residential buildings, *Wood products, Safety, Houses, Air pollution, Temperature, Humidity, Assessments, Concentration(Composition), *Indoor air pollution, *Air quality, *Consumer products.

The interim report describes procedures and presents results of the first phase of a laboratory project undertaken at the National Bureau of Standards for the Consumer Product Safety Commission (CPSC). The purpose of the ongoing project is to assess the accuracy of emission and indoor air quality models to be used by CPSC in predicting formaldehyde (HCHO) concentrations in residences due to pressed-wood products made with urea-formaldehyde bonding resins, namely particleboard underlayment, hardwood-plywood paneling and medium-density fiberboard (MDF). In phase

I, these products were characterized in 'medium-size' dynamic measuring chambers by measuring their HCHO surface emission rates over a range of HCHO concentrations, at 23C and 50% RH. They were then installed in a two-room prototype house and the equilibrium HCHO concentrations were monitored as a function of air exchange rate. Excellent agreement was obtained between measured HCHO concentrations and those predicted by a mass-balance indoor air quality model. In the next phase, the study will be repeated at various different temperatures and relative humidities so that models predicting HCHO surface emission rate as a function of temperature and humidity can be tested.

501,020

PB86-142403

Not available NTIS

National Bureau of Standards (NEL), Gaithersburg, MD. Building Physics Div.

Criteria and Design Guidelines for Reduced-Size Vents for One and Two Story Housing Units.

Final rept.,

R. Wyly, and L. S. Galowin. 1985, 26p

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

Pub. in ASPE Jnl. of Engineered Plumbing 1, n2 p97-122 Jul 85.

Keywords: *Residential buildings, *Plumbing, *Vents, Hydraulic test units, Measurement, Ventilation, Reprints.

The report describes hydraulic tests of drain-waste-vent systems with reduced-size vents installed in single-family housing units at Andrews Air Force Base, Camp Springs, Maryland. The vent systems of six field units were sized according to a procedure based on findings in prior laboratory investigations. The tests reported were conducted on three of the units before occupancy. Principal measurements made were trap-seal reduction and pneumatic pressure excursions in selected vents, using test procedures developed in the laboratory and adapted to field conditions. Results of the preoccupancy tests showed adequate performance with the reduced-size vents. A procedure for the design of reduced-size vent systems is presented that should be of interest to plumbing designers and groups engaged in updating plumbing codes.

501,021

PB86-153517

PC A04/MF A01

National Bureau of Standards (NEL), Gaithersburg, MD. Center for Applied Mathematics.

Paratransit Advanced Routing and Scheduling System Documentation: Functional Program and Data Specifications,

W. G. Hall, H. K. Hung, and R. E. Chapman. Dec 85, 61p NBSIR-85/3174

Sponsored by Urban Mass Transportation Administration, Washington, DC.

Keywords: *Urban transportation, Scheduling, Automation, *Paratransit, *Dial-a-ride systems, Routing, Computer applications, Control systems, Computer software, Central processing units.

The document specifies functional and data requirements governing automated procedures for routing and scheduling dial-a-ride vehicles. It provides overviews of existing methods and proposed methods, and summarizes improvements and impacts. Requirements for functions, performance, inputs-outputs, data characteristics, and failure contingencies are discussed fully. Three operating systems are specified. Finally, input and output data are described, and data collection procedures are presented.

501,022

PB86-166600

PC A03/MF A01

National Bureau of Standards (NEL), Gaithersburg, MD. Center for Building Technology.

Estimating Interroom Contaminant Movements,

G. N. Walton. Nov 85, 26p NBSIR-85/3229

Sponsored by Department of Energy, Washington, DC. Office of Building and Community Systems.

Keywords: *Ventilation, *Air pollution, Contaminants, Energy, Air flow, Circulation, Models, *Indoor air pollution, Computer applications.

Development of infiltration and interroom airflow calculation methods, driven by a concern for indoor air quality have led to a computer simulation of interroom contaminant movement. The model, which assumes fully

Field 13—MECHANICAL, INDUSTRIAL, CIVIL, AND MARINE ENGINEERING

Group 13B—Civil Engineering

mixed room air, shows that open doorways provide rapid mixing between rooms in buildings using forced air heating. It also confirms that it is most energy efficient to remove the contaminant nearest its source. Detailed modeling of the variations in contaminant concentration within a room is not presently feasible. The concept of ventilation effectiveness should provide sufficient accuracy and reasonable computing speed to be added to some existing energy analysis programs. Current energy analysis programs with long timesteps tend to run into convergence problems when solving the system performance and interroom airflows simultaneously. Short timestep simulation may be required. The need for computer modeling is demonstrated by the subtle behavior of a very simple system which removes contaminants by forced ventilation.

501,023

PB86-166626 PC A04/MF A01
National Bureau of Standards (NEL), Gaithersburg, MD. Building Physics Div.
Indoor Air Quality Modeling, Phase 1 Report. Framework for Development of General Models.
P. McNall, G. Walton, S. Silberstein, J. Axley, and K. Ishiguro. Oct 85, 65p NBSIR-85/3265
Sponsored by Environmental Monitoring Systems Lab., Research Triangle Park, NC.

Keywords: *Ventilation, *Air pollution, Models, Circulation, Development, Predictions, Formaldehyde, Radon, Nitrogen oxides, Smoke, Particulates, Carbon dioxide, Carbon monoxide, *Indoor air pollution.

The report presents a framework for the development of a model for predicting the indoor air pollutant concentrations in a variety of building types under practical conditions of weather, building occupancy, building construction and pollutant source strength. The general concepts needed for developing an indoor air quality model are treated. Examples of the current state of indoor air quality models are given. The pollutants discussed are formaldehyde, radon, nitrogen oxides, tobacco smoke, particulates, carbon dioxide, and carbon monoxide.

13C. Construction Equipment Materials, and Supplies

501,024

PB85-189199 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Structures Div.
Maturity Method: Theory and Application.
Final rept.,
N. J. Carino. 1984, 13p
Pub. in Cement, Concrete and Aggregates 6, n2 p61-73 1984.

Keywords: *Concretes, *Strength, Hardening(Materials), Theories, Mortars(Materials), Predictions, Thermodynamic properties, Temperature, Time, Reprints, *Maturity method, Arrhenius equation, Aging(Materials).

The maturity method may be used to predict the in-place strength of hardening concrete based on its thermal history. This paper presents a theoretical basis for the maturity method. The general form of the time-temperature function is found to be the time integral of the rate constant. For the case of linear dependence between temperature and the rate constant, the time-temperature function becomes the traditional maturity function. The Arrhenius equation is shown to be an accurate representation of the temperature dependence of the rate constant, and the concept of equivalent age is explained for practical application of the Arrhenius equation. It is explained how the accuracy of strength prediction by the traditional maturity method can be improved by using the proper datum temperature. Results illustrate that the appropriate value of apparent activation energy or datum temperature for concrete may be obtained from strength-gain data of isothermally-cured, mortar specimens.

501,025

PB85-189256 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Building Equipment Div.

Upgrading Plumbing Vent Systems in Rehab Buildings.

Final rept.,
L. S. Galowin, and F. Winter. Dec 84, 5p
Pub. in Heating/Piping/Air Conditioning 56, n12 p113-117 Dec 84.

Keywords: *Venting, *Buildings, *Plumbing, Circulation, Vents, Performance evaluation, Drains, Traps, Wastes, Reprints, *Retrofitting.

Rehabilitation, modernization, or renovation of existing buildings, as a resource to be conserved or recycled and reused, frequently imposes increased loads on the plumbing water supply and drainage system. An experimental laboratory investigation of 'circulation loop' modification to the drain-waste-vent (DWV) system to relieve the marginal performance of existing installations is reported. The experimental evaluations of the performance of the modified system and a conventional system were undertaken for a variety of wastewater load simulated conditions with various plumbing fixtures and multistory soil stack loads. The performance parameters considered were evaluation of trap seal failures and siphonic action of the water closets. Also, the dynamic responses to pressure excursions and air flow rate distributions in the branches were measured. Both systems were tested to the limiting condition for single-stack performance over a range of air flow variations into the soil and vent stack.

501,026

PB85-195311 PC A04/MF A01
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Building Technology.
Urea-Formaldehyde Foam Insulations: A Review of Their Properties and Performance.
Technical note (Final),
W. J. Rossiter, and R. G. Mathey. Mar 85, 74p NBS/TN-1210
Sponsored by Department of Energy, Washington, DC. Also available from Supt. of Docs as SN003-003-02641-7.

Keywords: *Thermal insulation, *Urea formaldehyde resins, Performance, Buildings, Standards, Cellular plastics, Properties, Energy conservation, Retrofitting, Indoor air pollution.

This report presents a review of the properties and performance of urea-formaldehyde foams pertinent to their use as thermal insulation for buildings. The review is based primarily on existing published literature. The factors affecting the performance of these insulations are listed and discussed. Included among these factors are durability, effect on energy conservation, effect on other building materials, fungus resistance, shrinkage, and temperature and humidity effects on foam. A key issue involving the use of urea-formaldehyde foam insulation is its release of formaldehyde, other gases, and particulates into the air of residences. Information concerning the release of these agents is summarized.

501,027

PB85-197655 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Effects of Maximum Void Size and Aggregate Characteristics on the Strength of Mortar.
Final rept.,
L. I. Knab, J. R. Clifton, and J. B. Ings. 1983, 8p
Pub. in Cement and Concrete Research 13, n3 p383-390 May 83.

Keywords: *Mortars(Materials), Voids, Aggregates, Flexural strength, Reprints.

The effects of the maximum void size and aggregate surface roughness and shape on the flexural strength of mortar were investigated. Substantial reductions in the maximum void size and air content of high strength quartz aggregate mortars resulted in flexural strength increases. However, these increases were lower than predicted by the Griffith theory, thus indicating that the maximum void size did not act as the critical flaw controlling the flexural strength. Rather, factors relating to the cement-aggregate bond, including aggregate roughness and surface area, appeared to affect the flexural strength more than the maximum void size.

501,028

PB85-200095 PC A03/MF A01
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Building Technology.

Alkali-Silica Reaction in Concrete.

Final rept. Nov 83-Jan 85,
L. J. Struble. Mar 85, 38p NBSIR-85/3116
Grant NSF-CEE82-10791

Keywords: *Concretes, *Alkalies, *Silicon dioxide, Portland cements, Aggregates, Cracks, Mortars(Materials), Tests, Chemical reactions.

Reaction in concrete between alkalies from the cement and reactive silica in the aggregate may cause expansion and cracking, and occasionally may cause significant weakening of the structure. The objective of this program is to determine whether there is any influence of the alkali mineralogy in the cement on the expansion of mortar due to alkali-silica reaction. The experimental approach consisted of determining the distribution of alkalies within a group of commercial portland cements with a variety of alkali mineralogies, and measuring expansion of mortar bars prepared using these cements and various reactive aggregates. In some cases, differences were observed in both level and rate of expansion for cements differing in alkali mineralogy. The differences were substantial with cements high in alkali and with opal as the reactive constituent. The results support the authors hypothesis that the specific alkali mineralogy of the cement affects the expansion due to alkali-silica reaction.

501,029

PB85-202117 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Impact Testing of Concrete.
Final rept.,
J. R. Clifton, and L. I. Knab. 1983, 8p
Sponsored by Defense Nuclear Agency, Washington, DC.
Pub. in Cement and Concrete Research 13, n4 p541-548 Jul 83.

Keywords: *Concretes, *Impact tests, Penetration, Projectiles, Impact strength, Latex, Compressive strength, Failure, Reinforced concrete, Steels, Reprints.

Three test methods were developed to determine the resistance of concrete subjected to low velocity single- and repeated impact to failure, and to higher velocity small projectiles. These performance tests were used to evaluate the effects of reinforcing concrete with one or more of the following reinforcement types: steel fibers, rebar or expanded metal. Concretes with and without latex were included.

501,030

PB85-224467 PC A05/MF A01
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Building Technology.
Assessment of Needs for New Thermal Reference Materials.
B. Rennex. May 85, 92p NBSIR-85/3146
Sponsored by Department of Energy, Washington, DC.

Keywords: *Calibrating, *Thermal measuring instruments, *Thermal insulation, Construction materials, Thermal measurements, Heat transfer, Thermal conductivity, Thermal resistance, Temperature.

Thermal insulation specimens are required by users to calibrate their heat transfer apparatuses. This report assesses the need for additional calibration specimens to cover a wider range of test conditions and materials. It examines two major sources of measurement error related to the use of calibration specimens. The first is due to the lack of uniformity over a specimen area and the second is due to systematic apparatus errors which vary with the values of specimen mean temperature and thermal conductivity. Possible solutions to these problems are given, based on information obtained from users in universities, industry, and government laboratories. These include recommendations to provide calibration specimens over a wide range of values of specimen temperature and thermal conductivity.

501,031

PB85-229862 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Inorganic Materials Div.
Fracture Toughness of Polymer Concrete Materials Using Various Chevron-Notched Configurations.
Final rept.,
R. F. Krause, and E. R. Fuller. 1984, 16p
Sponsored by Department of Energy, Washington, DC.

MECHANICAL, INDUSTRIAL, CIVIL, AND MARINE ENGINEERING—Field 13

Construction Equipment Materials, and Supplies—Group 13C

Pub. in American Society for Testing and Materials, Special Technical Publication 855, p309-323 1984.

Keywords: *Fracture strength, Acrylonitriles, Notch tests, Crack propagation, Reprints, *Polymer concretes, Stress intensity factors.

The fracture toughness of two similar polymer concrete materials was determined using several fracture mechanics configurations to show any influence of crack geometry on resistance to fracture in these materials. The testing configurations included a conventional straight-through notch in a flexure bar and various chevron-notched geometries in both flexure-bar and short-rod specimens. The materials were polymerized mixtures of monomers, anhydrous Type III portland cement, and silica sand. In one composition the monomers were styrene and trimethylolpropane-trimethacrylate; whereas, in the other composition, acrylonitrile was added as well. The fracture toughness was calculated from published stress-intensity coefficients for the straight-through notch which were adapted for use with a chevron notch by assuming that the derivative of the compliance with respect to crack length was the same for both notch types. Effects of varying chevron-notched angle, chevron-vertex position, and width of specimen in the crack plane were examined.

501,032
PB85-236024 PC A02/MF A01
National Bureau of Standards, Gaithersburg, MD.
Development of Durcon, an Expert System for Durable Concrete: Part 1,
J. R. Clifton, B. C. Oltkar, and S. K. Johnson. Jul 85, 24p NBSIR-85/3186

Keywords: *Concrete durability, *Concretes, Admixtures, Construction materials, Cements, Deterioration, Corrosion, Aggregates, Reinforcing steels, Sulfates, Mixtures, Design, Computer applications, Expert systems.

This is a progress report on the development of DURCON an expert system to give recommendations on the selection of constituents for durable concrete. Four major concrete deterioration problems will be covered when the DURCON system is completed; freeze-thaw, sulfate attack, corrosion of reinforcing steel, and cement-aggregate reactions. The factual knowledge base for DURCON is based on the American Concrete Institute Guide to Durable Concrete. Heuristic knowledge is being obtained from experts on the durability of concrete. The approach being taken in developing DURCON is discussed. Then a model expert system for concrete exposed to freeze-thaw conditions is described.

501,033
PB85-243715 PC A05/MF A01
National Bureau of Standards (NEL), Gaithersburg, MD. Building Materials Div.
Preliminary Recommendations for Maintenance of Factory Coated Metal Siding and Roofing,
M. C. McKnight, R. G. Mathey, and R. W. Drisko. Jun 85, 87p NBSIR-85/3193
Sponsored by Air Force Engineering and Services Center, Tyndall AFB, FL. Prepared in cooperation with Naval Civil Engineering Lab., Port Hueneme, CA.

Keywords: *Roofing, *Siding, *Maintenance, Coatings.

Recommendations and guidelines are presented for condition assessment and maintenance of the exterior surfaces of factory coated metal siding and roofing. The metal siding and roofing products commonly encountered on Air Force installations are addressed. The types of deterioration of metal buildings and appropriate methods of repair and maintenance procedures are related to the materials and construction practices used. The results of field observations of the condition of many types of coatings on metal siding and roofing in varying states of deterioration are reported. A quantitative condition assessment procedure was developed for exterior surfaces of metal buildings and consists of two parts. First, the condition of the siding and roofing of the building is evaluated using inspection forms, visual standards, and descriptions of levels of deterioration. In the second part, recommended maintenance procedures are determined using the evaluation data and analytical procedures which were developed. Visual standards and detailed coating failure descriptions were developed in order to identify and categorize the condition of the metal siding and roofing of buildings.

501,034
PB86-102225 PC A04/MF A01
Stanford Univ., CA. Dept. of Aeronautics and Astronautics.
Behavior of Furniture Frames during Fire.
Rept. for 1 Oct 83-30 Sep 84,
G. S. Springer. May 85, 58p NBS/GCR-85/494
Grant NB83-NADA-4019

Keywords: *Fires, *Furniture, Frames, Evaluation, Behavior, Tests, Wood products, Mathematical models, Mechanical properties, Strength, Fasteners, Failure, Temperature, Time measurement, Residential buildings, Construction materials, Fire tests, Computer applications.

The objective of the investigation is to evaluate the behavior of furniture frames during fire. Tests were performed measuring the strengths and deflections of wooden (southern pine) bends and joints exposed to elevated temperatures. The times to failure were also determined. A model was developed describing the strengths of wooden bends. Building on this model, a computer code was written which can be used to calculate the strengths of bends at room temperature. The code will serve as a basis for calculating the changes in strengths at elevated temperatures and for predicting the failure time.

501,035
PB86-111960 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Building Materials Div.
Prediction of Concrete Service-Life.
Final rept.,
J. Pommersheim, and J. R. Clifton. 1985, 10p
Pub. in *Materiaux et Constructions* 18, n103 p21-30 1985.

Keywords: *Concrete, *Life(Durability), *Mathematical models, *Accelerated tests, *Degradation, *Service life, Scale(Corrosion), Corrosion, Reprints.

The paper discusses development of accelerated tests and mathematical models for predicting the durability of concrete. Durability, service life, and degradation factors are defined and accelerated test methods are contrasted to conventional comparative methods. Factors and mechanisms of concrete degradation are reviewed, as are efforts to quantify these phenomena. Deterministic and stochastic models are discussed. Procedures for developing accelerated tests are presented and applied to a hypothetical example involving freeze-thaw damage. Advantages and disadvantages of accelerated testing and mathematical modeling are discussed in terms of the degradation mechanisms affecting concrete. Examples given of the modeling approach and service life prediction include the prediction of the strength and maturity of concrete, acid attack on cement, sulphate attack, and the effect of scaling and corrosion on load-bearing capacity of concrete.

501,036
PB86-114006 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Structures Div.
Stone Consolidating Materials.
Final rept.,
J. R. Clifton, and G. Frohnsdorff. 1982, 25p
See also PB80-202922.
Pub. in *Conservation of Historic Stone Buildings and Monuments*, p287-311 1982.

Keywords: *Consolidation, *Building stones, Performance evaluation, Service life, Construction materials, Field tests, Laboratory equipment, Reprints.

Mechanisms by which stone consolidants function are outlined. Evaluation of stone consolidants usually requires both laboratory and field tests to determine their initial and long-term performances. ASTM Standard E 632, Recommended Practice for Development of Accelerated Short-Term Tests for Prediction of the Service Life of Building Materials and Components, can be used to provide guidance on the test program. Materials which have been investigated as stone consolidants are reviewed. They fall into four main groups: inorganic materials, alkoxysilanes, synthetic organic polymers, and waxes. A universal stone consolidant does not exist, but epoxies, acrylics, and alkoxysilanes are the most commonly used consolidants.

501,037
PB86-128808 Not available NTIS

National Bureau of Standards (NEL), Gaithersburg, MD. Structures Div.
Corrosion Processes in Building Insulation Systems.

Final rept.,
J. M. Pommersheim, J. Lobo, and J. R. Clifton. 1981, 5p
Pub. in *Proceedings of International Conference Durability of Building Materials and Components* (2nd), Gaithersburg, MD., September 14-16, 1981, p274-278.

Keywords: *Corrosion, *Thermal insulation, Condensing, Buildings, Mathematical models.

The factors responsible for the corrosion of metal building service elements (such as electrical receptacle boxes and pipes) in contact with thermal insulation are discussed. The amount of corrosion and corrosion rate depend on the amount of condensation, the rate of drying and the leaching rate of impurities from the insulation.

501,038
PB86-133592 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Nondestructive Evaluation in Rehabilitation and Preservation of Concrete and Masonry Materials.
Final rept.,
J. R. Clifton. 1985, 11p
Sponsored by Construction Engineering Research Lab. (Army), Champaign, IL.
Pub. in *American Concrete Institute Special Publication* 85-2, *Rehabilitation, Renovation and Preservation of Concrete and Masonry Structures*, p19-29 1985.

Keywords: *Concretes, *Masonry, *Assessments, Nondestructive tests, Reinforcing materials, Buildings, Renovating, Evaluation, Reprints, *Preservation.

The paper describes nondestructive evaluation (NDE) methods that can be used in assessing the condition of concrete and masonry materials and components in structures being rehabilitated or preserved. Metal reinforcement is also included. The appropriate use of NDE methods is discussed and a recommended approach to selecting NDE methods for specific situations is given.

501,039
PB86-137924 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Structures Div.
Limit States Criteria for Masonry Construction.
Final rept.,
B. Ellingwood, and A. Tallin. 1985, 15p
Pub. in *Jnl. of Structural Engineering* 111, n1 p108-122 Jan 85.

Keywords: *Masonry cements, Masonry, *Brick construction, Construction materials, Criteria, Tests, Reprints.

Specifications for masonry and other construction materials are expected to move gradually over the next several years toward the adoption of probability-based limit states criteria for design. The paper illustrates how such criteria might be developed for brick and concrete masonry construction using, as an example, masonry walls loaded in combinations of axial compression and out-of-plane flexure. The paper shows the type of data that are necessary and how that data can be manipulated within the probabilistic framework to develop probability-based resistance criteria.

501,040
PB86-169109 PC A99/MF E04
National Bureau of Standards, Gaithersburg, MD. Ceramics Div.
Construction Materials for Coal Conversion: Performance and Properties Data. Supplement 2.
Final rept.,
H. M. Ondik. Dec 85, 695p NBS/SP-642-SUPPL-2
See also PB84-165331. Also available from Supt. of Docs as SN003-003-02703-1. Library of Congress catalog card no. 85-600639.

Keywords: *Construction, *Coal gasification, *Ceramics, Industrial plants, Alloys, Mechanical properties, Physical properties, Performance evaluation, Failure, Corrosion, Erosion, Tables(Data), Equipment, Refractories, Coal liquefaction.

The book expands the information provided in the original NBS/SP 642 and in NBS/SP 642 Supplement 1 publications, *Construction Materials for Coal Conversion*.

Field 13—MECHANICAL, INDUSTRIAL, CIVIL, AND MARINE ENGINEERING

Group 13C—Construction Equipment Materials, and Supplies

sion--Performance and Properties Data. These volumes are intended to provide a central source of materials information needed for the fossil fuel industry. Data have been collected and evaluated from Department of Energy-sponsored projects. The book is organized so that the information is given both with respect to the various component areas of coal gasification, liquefaction, and direct combustion plants and also with respect to the properties or possible failure mechanisms, e.g., corrosion, erosion, mechanical properties, and physical properties.

13D. Containers and Packaging

501,041
PB86-108776 PC A06/MF A01
National Bureau of Standards, Gaithersburg, MD.
Package Checking Field Manual to Accompany NBS (National Bureau of Standards) Handbook 133: Checking the Net Contents of Packaged Goods.
C. S. Brickenkamp, S. Hasko, and M. G. Natrella.
Aug 85, 107p NBSIR-85/3172
See also PB85-129153.

Keywords: *Handbooks, *Packaging, Sampling, Inspection, Measurement, Procedures, Computation, Compliance.

Tables and report forms from NBS Handbook 133 have been rearranged in a convenient tabbed format for use by government inspectors in their field testing of prepackaged consumer and nonconsumer commodities. Outlines of the test procedures and examples of completed report forms and worksheets have been added, along with a variation on the 'Standard Pack Report Form' for weight only. There are eight sections: Test Procedure Outlines, Sampling Plans, Variable Tare, Weighing Rules, MAV's, Report Forms and Worksheets, Examples, and a Random Number Table.

13E. Couplings, Fittings, Fasteners, and Joints

501,042
PATENT-4 559 717 Not available NTIS
Department of Commerce, Washington, DC.
Flexure Hinge.
Patent,
F. E. Scire, and C. Teague. Filed 21 Feb 84,
patented 24 Dec 85, 10p PB86-141090, PAT-APPL-
6-581 831
Supersedes PB84-178557.
This Government-owned invention available for U.S. licensing and, possibly, for foreign licensing. Copy of patent available Commissioner of Patents, Washington, DC 20231 \$1.00.

Keywords: *Hinges, *Patents, Flexing, PAT-CL-33-568.

The invention relates to improved flexure devices as well as to the use of such devices in instrument stages capable of independent movement in each of two orthogonally-related dimensions. More particularly, the invention relates to an instrument stage having an output device form capable of independent xy motion in a single plane and which is virtually free of pitch, roll and yaw and of motion perpendicular to the plane of motion.

501,043
PB85-187326 Not available NTIS
National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.
Fitness-for-Service Criteria for Pipeline Girth-Weld Quality.
Final rept.,
R. P. Reed, M. B. Kasen, H. I. McHenry, C. M. Fortunko, and D. T. Read. Jul 84, 80p
See also PB84-165448. Sponsored by Department of Transportation, Washington, DC. Office of Pipeline Safety Regulation.
Pub. in Proceedings of Welding Research Council Bulletin No. 296, 80p Jul 84.

Keywords: *Welded joints, *Pipelines, Weld defects, Quality assurance, Criteria, Nondestructive tests, Ultrasonic tests, Crack initiation, Fatigue(Materials), Inspection, Acceptability, Weldments, Reprints.

Criteria have been developed for applying fitness-for-service analyses to flaws in girth welds. A critical crack-opening-displacement elastic-plastic fracture mechanics model was developed and experimentally verified. Procedures for constructing flaw acceptance curves based on this model are provided. A significantly improved ultrasonic method for detecting and dimensioning significant weld flaws was developed. The probability of crack initiation from blunt flaws was shown to be very low under severe low-cycle fatigue. Suggestions are offered for technical implementation of field inspection procedures and for practical implementation of the flaw acceptance criteria.

501,044
PB85-196095 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Serviceability Limit States - Connection Slip.
Final rept.,
T. V. Galambos, T. A. Reinhold, and B. Ellingwood.
1982, 13p
Pub. in Jnl. of the Structural Division, American Society of Civil Engineers 108, n12 p2668-2680 Dec 82.

Keywords: *Service life, *Joints(Junctions), Mechanical properties, Probability theory, Statistical analysis, Bolted joints, Limits, Design criteria, Resistance, Steels, Reprints, *Slip.

The serviceability limit state for slip of bolted steel joints is the slip-resistance. The statistical properties of the parameters which define this resistance are presented and discussed. Based on these properties and using First-Order Second-Moment probabilistic analysis, limit-states design criteria are developed for friction-grip bolted joints.

501,045
PB85-207371 Not available NTIS
National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.
Nonmetallic Composites in Space Dewars.
Final rept.,
M. B. Kasen. 1984, 9p
Pub. in Proceedings of 1983 Space Helium Dewar Conf., Huntsville, AL., August 24-26, 1984, p171-179.

Keywords: *Dewar flasks, *Composite materials, Pressure vessels, Epoxy matrix composites.

A review of past and present usage of nonmetallic composites in cryogenic dewars and pressure vessels is presented. Particular attention is paid to the extent to which advances in cryogenic composite technology offer new approaches to fabricating thermally efficient systems. It is concluded that more efficient dewar support members can be fabricated by correct utilization of materials in particular temperature ranges. It is further concluded that fabrication of improved cryogenic container vessels is possible utilizing current knowledge of the factors influencing cryogenic performance under thermal and mechanical cyclic loading.

501,046
PB85-208007 Not available NTIS
National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.
Monocrystal Elastic Constants in the Ultrasonic Study of Welds.
Final rept.,
H. M. Ledbetter. Jan 85, 5p
Sponsored by National Science Foundation, Washington, DC.
Pub. in Ultrasonics 23, p9-13 Jan 85.

Keywords: *Welded joints, *Ultrasonic tests, Elastic properties, Reprints.

For studying welds ultrasonically, the importance of knowing the material's single-crystal elastic constants, the C sub ijs, is explained. Where these constants are not known, some guidelines are given for estimating them from polycrystalline elastic constants such as Young's modulus and the shear modulus. The important case of (001) fiber texture is considered. Being transversely isotropic, the case exhibits five macroscopic elastic constants, which are related to the three cubic elastic constants: Csub 11, Csub 12, Csub 44. From the five constants the angular variations of Young's modulus, the torsional modulus, and the sound velocities can be computed. For the same (001)

fiber texture, results are given for a standard well-characterized material--copper, where the C sub ijs are well known.

501,047
PB85-227098 PC A04/MF A01
National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.
Ductile-to-Brittle Transition In Steel Weldments for Arctic Structures.
F. Zia-Ebrahimi. Apr 85, 66p NBSIR-85/3020
Sponsored by Minerals Management Service, Reston, VA.

Keywords: *Weldments, *Welded joints, Fracture properties, Steels, Ductile brittle transition, Cold weather construction, Microstructure, Crack initiation.

The report summarizes the work performed in support of the development of fracture criteria for steel weldments in arctic structures. The ductile-to-brittle transition behavior of a shielded metal-arc weld, typical of steel weldments in arctic structures, has been studied. Fracture toughness, Charpy V-notch impact energy, and tensile properties have been measured as a function of temperature throughout the ductile-to-brittle transition range. The effect of geometric dimensions on fracture toughness has been studied for three geometries of single-edge-notch-bend (SENB) specimens. The fracture surfaces of broken specimens have been characterized by scanning electron microscopy (SEM). The microstructure of the multiple-pass weldment has been studied by optical microscopy. The mechanical properties of the steel weldment have been compared to the base metal, an ABS grade EH36 steel in normalized condition.

501,048
PB85-237121 PC A05/MF A01
National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.
Experimental Results for Fitness-for-Service Assessment of HY130 Weldments.
Final rept. Oct 81-Sep 82,
D. T. Read. Mar 84, 95p NBSIR-84/1699
Sponsored by Naval Sea Systems Command, Washington, DC.

Keywords: *Weldments, *Quality assurance, Assessments, Welded joints, Steels, Cracks, Residual stress, Steel HY130, Fracture(Mechanics), J integrals.

Applied J-integral values for through and surface cracks in HY130 weldments and for surface cracks in HY130 base metal have been measured using a previously developed technique. The applied J-integral is taken as a measure of the crack driving force. The results confirmed previous conclusions, namely, the strong effect of deformation pattern on applied J-integral values, the utility of the J-integral estimation curve for fitness-for-service assessment in cases of gross section yielding (crack size less than 1 percent of load-bearing cross-section), and the need to consider ligament yielding behind surface cracks.

501,049
PB86-124823 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Inorganic Materials Div.
Development of Some Analytical Fracture Mechanics Models for Pipeline Girth Welds.
Final rept.,
R. de Wit, and J. H. Smith. 1980, 16p
Sponsored by Department of Transportation, Washington, DC. Office of Pipeline Safety Regulation.
Pub. in American Society for Testing and Materials, Special Technical Publication 700, p513-528 1980.

Keywords: Fracture properties, *Pipelines, *Welded joints, Mechanical properties, Cracking(Fracturing), Failure, Defects, Reprints, *Fracture(Mechanics).

Fracture mechanics methods have been used to provide a basis for assessing the significance of defects in pipeline girth welds. Analytical models based on fracture mechanics technology are developed to establish predicted critical defect sizes for sharp, circumferential defects in pressurized pipe. The general problem considered here is that of a surface defect in a plate, i.e. they use the flat plate analogy for a pipeline. Failure is considered to occur when the ligament ruptures and provides a leakage path. The fracture mechanics model used, called the collapsed ligament model, is based on the work of Erdogan and Bakioglu which is in turn based on the Dugdale model. The collapsed liga-

ment model assumes plastic collapse in the depth direction, but any fracture mechanics model in the length direction.

501,050
PB86-139862 Not available NTIS
National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.

Texture in Stainless Steel Welds: An Ultrasonic Study.

Final rept.,
H. M. Ledbetter, and M. W. Austin. 1985, 5p
Pub. in Jnl. of Materials Science 20, p1720-1724 1985.

Keywords: *Weldments, *Ultrasonic tests, Stainless steels, Texture, Elastic properties, Steel 316.

The authors studied texture effects in five AISI-316 stainless-steel welds. The authors measured nine independent ultrasonic velocities along the weld's principal axes. These velocities reveal a strong texture different from the <001> fibre-type usually attributed to these materials.

13H. Industrial Processes

501,051
PB85-177905 PC A03/MF A01
Illinois Univ. at Urbana-Champaign. Dept. of Civil Engineering.
Mapping Principles for the Standards Interface for Computer Aided Design,
L. A. Lopez, and S. L. Elam. Feb 85, 40p NBSIR-85/3115

Keywords: *Building codes, *Design standards, Mapping, Construction, Data processing, *Computer aided design, Analysis, Data bases.

Integrated computed aided design has great potential for increasing the quality and efficiency of the design process. However, building designs are subject to requirements expressed in standards (including project-specific criteria, specified national standards and building codes). Standards must be incorporated correctly and efficiently in the computer aided design process in order that the process be correct and efficient. Standards must be programmed for data processing, checked for consistency with the project and legal requirements, and updated when these requirements are changed or updated. Programs for standards, applications programs for design, and project data bases should be distinct, but integrable, to permit each to be developed independently, but then to be widely applicable in association with other programs. Techniques developed for standards analysis, synthesis and expression (SASE) are extended to allow SASE representations of standards to serve as programs expressing the standards for use in computer aided design. Mapping principles are derived to define the data interface requirements between SASE representations of standards and applications programs.

501,052
PB85-187821 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Sensory Interactive Control Systems for Advanced Manufacturing.

Final rept.,
G. J. Vanderbrug, J. S. Albus, and A. J. Barbera. 1980, 9p
Sponsored by International Federation of Automatic Control, Laxenburg (Austria) and International Federation for Information Processing, Geneva (Switzerland).
Pub. in Proceedings of Information Control Problems in Manufacturing Technology, IFAC/IFIP Symposium (2nd), Stuttgart, Germany, October 22-24, 1979, p137-145 1980.

Keywords: *Robots, *Control equipment, Detectors, Manufacturing, Interactive systems, Robot vision.

Fundamental understanding of sensory interactive control systems is an important step in applying advanced manufacturing techniques. Functional requirements and an architecture for a sensory interactive robot control system are presented. A model for studying the interaction between the control and sensory parts of a system is presented. The model consists of parallel control decomposition and sensory analysis hierarchies. A robot vision system is described, with

special emphasis on the nature of its interaction with the control part of the system.

501,053
PB85-196160 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Acoustic-Emission-Monitored Tests for TAB Inner Lead Bond Quality.

Final rept.,
G. G. Harman. 1982, 9p
Sponsored by Department of Energy, Washington, DC. Energy Information Administration, and Components, Hybrids and Manufacturing Technology Society (IEFE), New York.
Pub. in Proceedings of Electronic Components Conference (32nd), San Diego, CA, May 10-12, 1982, p268-276.

Keywords: Quality, Integrated circuits, Semiconductor devices, Bonding, Fatigue tests, Nondestructive tests, *Acoustic emission testing.

The paper gives a brief introduction to acoustic-emission (AE) based tests applied to quality control in the electronics industry and describes some recent research on this testing technique. Equipment and circuits are described that may be used to implement such AE-monitored testing. Acoustic-emission monitored tests to determine the inner lead bond quality for Tape Automated Bonding (TAB) have been developed. These include a pull tester and a microfatigue tester for off-line evaluation of bond quality and metallurgical system reliability as well as an automatic on-line production bond quality tester. The microfatigue tester for TAB leads can apply a small oscillatory (up to 80 Hz) force on top of a constant force bias of a few grams.

501,054
PB85-230399 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.

Ultrasonic Measurement of Solid/Liquid Interface Position during Solidification and Melting of Iron and Steel.

Final rept.,
R. L. Parker. 1984, 4p
See also PB83-139170.
Pub. in Proceedings of the Symposium on Application and Development of NDE for Use in Materials Processing, Philadelphia, Pennsylvania, October 3-4, 1983, p23-25 1984.

Keywords: *Ultrasonic tests, *Interfaces, Iron, Steels, Melting, Solidification, Measurement, Process control.

The solidification and melting of iron and stainless steel have been studied using a pulse-echo ultrasonic flaw detector, with longitudinal waves between 1 and 10 MHz. The change in acoustic impedance at the solid/liquid interface causes a portion of the beam energy to be reflected.

501,055
PB85-233823 CP T03
National Bureau of Standards (NEL), Gaithersburg, MD. Factory Automation Systems Div.

Hierarchical Control System Emulator Version 3.1.
Model-Simulation,
C. Furlani. Jul 85, mag tape NBS/SW/MT-85/003
Supersedes PB85-152759.
Source tape is in the ASCII character set. This restricts preparation to 9 track, one-half inch tape only. Identify recording mode by specifying density only. NTIS Computer Products if you have questions. Price includes documentation, PB85-233849, PB85-233831, and PB83-175075.

Keywords: *Models-simulation, *Control simulation, *Automatic control, Computerized simulation, Magnetic tapes, Real time operations, Industrial plants, Production control, Automation, Fortran, *Hierarchical control, Emulators(Computers), *Control systems, *Computerized control systems, *Computer aided design, Computer aided manufacturing, Praxis programming language, VAX-11/780 computers.

The Hierarchical Control System Emulator is a collection of computer programs written in the high-level Praxis language for use on a Digital Equipment Company VAX 11/780(TM) processor under the VMS(TM) operating system. The programs allow the user to write, debug, and concurrently emulate modules of a hierarchical control system and to simulate the physical plant which is controlled. The emulation executes in real time and interactive display and data logging

capabilities are included. The emulator is currently implemented at the NBS Automated Manufacturing Research Facility as a computer-aided control system design tool. The magnetic tape contains a copy of version 3.1 of the entire HCSE software package. In addition, the tape is accompanied by an instruction sheet which describes the procedure for transferring the HCSE from magnetic tape to a VAX/VMS system. Software Description: The Model is written in the FORTRAN programming language for implementation on a Digital Vax-11/780 computer using the Vax/VMS V.3.7 operating system.

501,056
PB85-233831 PC A03/MF A01
National Bureau of Standards (NEL), Gaithersburg, MD. Factory Automation Systems Div.

Hierarchical Control System Emulation Programmer's Manual,

C. M. Furlani. Jan 85, 48p NBSIR-85/3157, NBS/SW/MT-85/003B
Supersedes PB83-137059. For system on magnetic tape, see PB85-233823.

Keywords: *Control simulation, *Automatic control, Programming manuals, Computerized simulation, Real time operations, Industrial plants, Production control, Automation, Fortran, *Hierarchical control, *Control systems, *Computerized control systems, *Computer aided design, Computer aided manufacturing, Emulators(Computers), VAX-11/780 computers, Praxis programming language.

The Hierarchical Control System Emulation is a collection of computer programs written in the high-level Praxis language for use on a Digital Equipment Company VAX 11/780(TM) processor under the VMS(TM) operating system. The programs allow the user to write, debug, and concurrently emulate modules of a hierarchical control system and to simulate the physical plant which is controlled. The emulation executes in real time and interactive display and data logging capabilities are included. The emulation is intended as a computer-aided control system design tool for the NBS Automated Manufacturing Research Facility. The Programmer's Manual provides documentation of the design of the emulation code and the emulation programs themselves; it is intended for the system programmer rather than the user.

501,057
PB85-233849 PC A07/MF A01
National Bureau of Standards (NEL), Gaithersburg, MD. Factory Automation Systems Div.

Hierarchical Control System Emulation User's Manual,

C. M. Furlani. Jan 85, 136p NBSIR-85/3156, NBS/SW/MT-85/003A
Supersedes PB83-141952. For system on magnetic tape, see PB85-233823.

Keywords: *Control simulation, *Automatic control, Computerized simulation, Real time operations, Industrial plants, Production control, Automation, Fortran, *Hierarchical control, *Control systems, *Computerized control systems, *Computer aided design, Computer aided manufacturing, Emulators(Computers), Praxis programming language, User manuals.

The Hierarchical Control System Emulation is a collection of computer programs written in the high-level Praxis language for use on a Digital Equipment Company VAX 11/780(TM) processor under the VMS(TM) operating system. The programs allow the user to write, debug, and concurrently emulate modules of a hierarchical control system and to simulate the physical plant which is controlled. The emulation executes in real time and interactive display and data logging capabilities are included. The emulation is intended as a computer-aided control system design tool for the NBS Automated Manufacturing Research Facility. The User's Manual describes the use of the emulation and provides necessary theoretical background; it is not application-specific.

501,058
PB86-106754 PC A05/MF A01
Michigan Univ., Ann Arbor. Graduate School of Business Administration.

Survey of the Literature on Production Scheduling as It Pertains to Flexible Manufacturing Systems,
N. Raman. Aug 85, 89p NBS/GCR-85/499
Sponsored by National Bureau of Standards (NEL), Gaithersburg, MD. Center for Applied Mathematics.

Field 13—MECHANICAL, INDUSTRIAL, CIVIL, AND MARINE ENGINEERING

Group 13H—Industrial Processes

Keywords: *Reviews, *Production control, Manufacturing, Automation, Robots, Industrial plants, Production engineering, *Flexible manufacturing systems, Computer aided manufacturing.

The paper presents a survey of the existing literature on machine scheduling from the perspective flexible manufacturing systems. It is the first of a series of papers planned to document research in scheduling for the Automated Manufacturing Research Facility (AMRF) at the National Bureau of Standards. An overview of the hierarchical production planning process is given. The paper covers deterministic, non-preemptive scheduling of open shops, since a typical flexible manufacturing system (FMS) operates under these conditions. Both due-date based and flow-time based objectives are addressed for single stage single machine, single stage parallel machines, flow shops and job shops. Research in assembly line balancing is similarly covered since it is possible to treat an FMS as a transfer line for repetitive discrete manufacture. The analytical approaches to these problems have focussed primarily on the objectives of maximizing production rate, minimizing in-process inventory, and maximizing machine utilization.

501,059

PC A04/MF A01

Michigan Univ., Ann Arbor. Graduate School of Business Administration.

Simulation Model for the Automated Manufacturing Research Facility,

N. Raman. Aug 85, 55p NBS/GCR-85/498

Sponsored by National Bureau of Standards, Gaithersburg, MD.

Keywords: *Industrial plants, *Manufacturing, Mathematical models, Automation, Robots, Production control, *Computer aided manufacturing, Microcomputers, Discrete event system, SIMAN programming language.

The paper presents a simulation model for investigating and validating the operating policies of the Automated Manufacturing Research Facility (AMRF) at the National Bureau of Standards for the June 1985 configuration. The model is written in SIMAN, and runs on any microcomputer which can be run under the MS-DOS operating system. The model represents the AMRF as a discrete-event system and consists of two segments. The values of the system parameters are presented in the Experimental Frame segment. The output includes pertinent statistics such as utilization of each workstation, number of jobs waiting at each workstation, average flow time and average tardiness of jobs of each part type. Procedures for interfacing the simulation output with the LOTUS 1-2-3 graphics package are also included. The impact of different operating policies and scheduling rules can be studied by making relatively minor changes in the Block Diagram. Alternatively, the effect of altering the values of the system parameters can be investigated by making suitable changes in the Experimental Frame.

501,060

PC A10/MF A01

National Bureau of Standards, Gaithersburg, MD. Office of Product Standards Policy.

Private Sector Product Certification Programs in the United States.

Final rept., M. A. Breitenberg. Aug 85, 225p NBS/SP-703

Also available from Supt. of Docs as SN003-003-02673-5. Library of Congress catalog card no. 85-600574.

Keywords: *Directories, *Product development, *Quality control, Standards, United States, Inspection, Specifications, Programs, *Certification.

The directory presents information from 109 private sector organizations in the United States which engage in product certification activities. Entries describe the type and purpose of each organization, the nature of the activity, products certified, standards used, certification requirements, availability and cost of services, and other relevant details. This directory is part of an ongoing NBS effort to establish and maintain a comprehensive database on standards, regulations, certification programs and related information. This material has been compiled to meet the needs of government, industry, and the public for information on private sector product certification programs in accordance with the requirements of the U.S. Trade Agreements Act of 1979.

501,061

Not available NTIS

National Bureau of Standards, Gaithersburg, MD. Inorganic Materials Div.

Immersion Deposition Process.

Final rept., D. S. Lashmore. 1982, 37p

Sponsored by Aluminum Association, Inc., Washington, DC., and American Electroplaters' Society, Inc., Winter Park, FL.

Pub. in Proceedings of Aluminum Finishing Seminar, St. Louis, MO., March 30-April 1, 1982, p501-537.

Keywords: *Electrodeposition, Surface finishing, Emersion, Plating, Aluminum, Stannates, Coatings, Etching, Substrates.

The immersion deposition process for plating on aluminum will be reviewed with emphasis on recent findings concerning the deposition mechanisms. Both the zincate types of processes as well as the stannate types of processes will be discussed. Included in the text is a discussion of the role of the etching pretreatment, reasons for double zincating, morphology of the coating and relationship between coating morphology and substrate morphology, and finally a discussion of the reason why certain metals adhere well to aluminum while others adhere poorly.

501,062

Not available NTIS

National Bureau of Standards (NEL), Gaithersburg, MD. Industrial Systems Div.

Virtual Manufacturing Cell.

Final rept., C. R. McLean, H. M. Bloom, and T. H. Hopp. 1983, 9p

Pub. in Proceedings of the IFAC/IFIP Symposium on Information Control Problems in Manufacturing Technology 1982 (4th), Gaithersburg, MD., October 26-28, 1982, p207-215 1983.

Keywords: *Production control, *Manufacturing, Automation, Routing, Scheduling, Artificial intelligence, Machining, *Computer aided control systems, Computer files, National Bureau of Standards.

A virtual manufacturing cell is being developed at the National Bureau of Standards as part of the control software for the Automated Manufacturing Research Facility (AMRF) project. The traditional group technology cell has evolved from the need to provide the flexibility to manufacture a family of parts while maintaining the efficiency associated with a single process flow line. Group technology cells normally require a fixed physical grouping of machining workstations for each class of parts. A shop based upon virtual manufacturing cells provides greater flexibility than existing shop configurations through the time sharing of machining workstations. Virtual cells are not identifiable as fixed physical groupings of machinery, but as data files and processes in the control computer. Given this structure, the shop level control system must now schedule the activation of job cells and the allocation of workstations to these cells. In this configuration, a workstation will always be under the control of a particular virtual cell or a pool cell (that is composed of idle, untasked workstations). Functions that the virtual cell will perform include analysis, reporting, routing, scheduling, dispatching, and monitoring.

501,063

Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

Electrical Test Structures for Characterization and Control of Microelectronics Processing.

Final rept., M. A. Mitchell, L. W. Linholm, T. J. Russell, and G. P. Carver. 1981, 29p

Pub. in Proceedings of Annual Seminar on Microelectronics Measurement Technology (3rd), San Jose, CA., March 17-18, 1981, v6 p1-29.

Keywords: *Microelectronics, *Test equipment, Electronics industry, Integrated circuits, Measurement, Materials, Production control, Control equipment, Performance evaluation, Reprints.

The trend toward smaller devices in larger integrated circuits makes assurance of product functionality increasingly difficult. The results of measurements from specially designed microelectronic test structures can be a critical ingredient in process characterization and control, two of the primary factors affecting circuit functionality. Test structures can be used to evaluate

IC materials, to evaluate and control process uniformity, to measure and control device and circuit parameters, to quantify the occurrence of process-related random faults, and to evaluate processing equipment performance. Electrical test structures and test methodologies reviewed here have been developed for rapid automated measurement of a variety of parameters. Simple, fast, visual correlations of the parameters in the form of wafer maps provide information about yield-reducing variations in parameters. Examples of such correlations are discussed.

501,064

Not available NTIS

National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.

Interface Depth Resolution of Auger Sputter Profiled Ni/Cr Interfaces: Dependence on Ion Bombardment Parameters.

Final rept., J. Fine, P. A. Lindfors, M. E. Gorman, R. L. Gerlach, and B. Navinsek. 1985, 5p
Pub. in Jnl. of Vacuum Science and Technology A3, n3 p1413-1417 May/June 85.

Keywords: *Sputtering, *Interfaces, Thin films, Depth, Width, Nickel, Chromium, Ion beams, Reprints, Auger spectroscopy.

Interface broadening which often results as a consequence of sputter profiling can make it difficult to assess the structure of an original interface. There are a number of factors involved in this broadening which are associated with the parameters of the ion bombardment and which have not previously been evaluated. Sputter profile measurements obtained on a set of similarly fabricated Ni/Cr multilayered thin-film structures have shown that it is practical to systematically examine this interface broadening dependence on ion beam energy, ion current density, and angle of incidence, all as a function of sputtered depth. Results are presented of such a set of Auger sputter depth profile measurements and indicate that there can be dramatic changes in sputtered interface widths depending on the ion bombardment parameters used.

501,065

Not available NTIS

National Bureau of Standards (NEL), Gaithersburg, MD. Center for Mfg. Engineering.

National Bureau of Standards' Automation Research Program.

Final rept., J. A. Simpson. 1983, 5p
Pub. in Proceedings of IFAC/IFIP Symposium (4th) on Information Control Problems in Manufacturing Technology, Gaithersburg, MD., October 26-28, 1982, p9-13 1983.

Keywords: *Standards, *Industrial plants, Automation, Machine tools, Process control, *Flexible manufacturing systems, *Research facilities, Computer aided manufacturing.

The program focuses on two problems lying close to the core mission of the National Bureau of Standards. First, how will the automated factory ensure that its products are dimensionally compatible with national standards. Second, what new national standards must be developed by the private sector to permit the increased productivity promised by automation to be realized in a free market economy. To explore these problems, an extremely flexible manufacturing research facility, with hierarchical, highly modular control architecture is being installed. This facility is designed to be capable of emulating a wide variety of manufacturing cells typical of a small machine shop.

501,066

Not available NTIS

National Bureau of Standards (NEL), Gaithersburg, MD. Automated Production Technology Div.

Rational Approach to Deburring for Flexible Manufacturing Systems.

Final rept., C. A. Wan. 1982, 18p
Pub. in Proceedings of AUTOFACT 4 Conference, Philadelphia, PA., November 30-December 2, 1982, p7.54-7.71.

Keywords: *Adaptive systems, *Deburring, Automatic control, Robots, Machine tools, Manufacturing, Tool life, *Flexible manufacturing systems, Computer aided manufacturing.

No abstract available.

501,067
PB86-140266 Not available NTIS
National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.
EMAT (Electromagnetic-Acoustic Transducer) Synthetic Aperture Approach to Thick-Weld Inspection.
Final rept.,
R. E. Schramm, and J. C. Moulder. 1985, 8p
Sponsored by Naval Sea Systems Command, Washington, DC.
Pub. in Review of Progress in Quantitative Nondestructive Evaluation, v4A p225-232 1985.

Keywords: *Nondestructive tests, *Ultrasonic tests, Inspection, Weldments, Transducers, Ultrasonic frequencies, Signal to noise ratio, Computer applications.

The paper describes developments in a system based on electromagnetic-acoustic transducers (EMATs) as an approach to automated nondestructive evaluation of thick weldments. Good signal-to-noise ratios, were possible through careful design of the transducers and associated electronic circuits and the use of signal averaging. At 454 kHz, the transducers produce shear-horizontal waves of approximately 7-mm wavelength in steel. The long wavelength permits determination of through-thickness flaw depth from the amplitudes of scattered ultrasonic waves. A minicomputer controlled transducer positioning and acquired the digitized ultrasonic waveforms for synthetic aperture processing. The synthetic aperture technique further improved signal quality and yielded flaw localization through the weld thickness.

13I. Machinery and Tools

501,068
PB85-182707 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Analysis of Robot Performance Operation.
Final rept.,
N. G. Dagalakis. 1983, 23p
Sponsored by Robotics International, Dearborn, MI.
Pub. in Proceedings of International Symposium on Industrial Robots and Robots 7 (13th), Chicago, IL., April 17-21, 1983, Applications Worldwide, v1 p 7.73-7.95.
Keywords: *Robots, Performance, Detection, Defects.

The use of two techniques for the detection of the presence of defects in robot arms was investigated. Two different types of defects were simulated on a PUMA 600 robot. A defect on the operation of the robot wrist joint controller and loosening of the robot end effector. Both techniques were able to detect the presence of the defects. Ways are suggested for determining the seriousness of each defect. At least in the case of the end effector loosening, the nature and seriousness of the defect seem to be easy to determine.

501,069
PB85-182830 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Six-Dimensional Vision System.
Final rept.,
J. Albus, E. Kent, M. Nashman, P. Mansbach, and L. Palombo. 1982, 12p
Sponsored by Computer Society (IEEE), Los Alamitos, CA., and Society of Photo-Optical Instrumentation Engineers, Bellingham, WA.
Pub. in Proceedings of SPIE Technical Symposium East '82, 336 p142-153 1982.

Keywords: Robots, Cameras, *Robot vision, Six degrees of freedom.

There are six degrees of freedom that define the position and orientation of any object relative to a robot gripper. All six need to be determined for the robot to grasp the object in a uniquely specified manner. A robot vision system under development at the National Bureau of Standards is designed to measure all six of these degrees of freedom using two frames of video data taken sequentially from the same camera position. The system employs structured light techniques; in the first frame, the scene is illuminated by two parallel planes of light, and in the second frame by a point source of light.

501,070
PB85-182848 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Architecture for Real-Time Sensory-Interactive Control Robots in a Manufacturing Facility.
Final rept.,
J. S. Albus, C. R. McLean, A. J. Barbera, and M. L. Fitzgerald. 1983, 10p
Sponsored by International Federation of Automatic Control, Laxenburg (Austria).
Pub. in Proceeding of the IFAC/IFIP Symposium, Gaithersburg, MD., October 26-28, 1982, Information Control Problems in Manufacturing Technology 1982, p81-90 1983.

Keywords: *Control equipment, *Robots, Detectors, Control theory, *Interactive control, Real time, Hierarchies.

A hierarchical architecture is described for a robot integrated into a real-time sensory interactive factory control system. In this architecture, high level goals are decomposed through a succession of levels, each producing strings of simpler commands to the next lower level. The bottom level generates the drive signals to the robot actuators. Each control level is a separate process with a limited scope of responsibility. Each performs the generic control function of sampling its input and generating appropriate outputs. The input is characterized by three types of data - a command from the next higher level, processed sensory data, and status feedback from the next lower level. The outputs are of three types - a command to the next lower level, a request for sensory information to the processing module at the same level, and a status feedback to the next higher level. This paper describes this generic control structure and its implementation in a real-time sensory-interactive control system for a manufacturing facility.

501,071
PB85-182871 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Concepts for a Real-Time Sensory-Interactive Control System Architecture.
Final rept.,
A. J. Barbera, M. L. Fitzgerald, and J. S. Albus. 1982, 6p
Sponsored by Virginia Polytechnic Inst. and State Univ., Blacksburg. Dept. of Electrical Engineering, and Computer Society (IEEE), Los Alamitos, CA.
Pub. in Proceedings of Annual Southeastern Symposium on System Theory (14th), Blacksburg, VA., April 15-16, 1982, p121-126.

Keywords: *Control equipment, *Feedback control, Robots, Real time, *Interactive control, Hierarchies.

The paper describes concepts used in defining an architecture for a real-time sensory-interactive control system. These concepts were arrived at from testing and evaluating different control system strategies at the National Bureau of Standards. A hierarchical task decomposition architecture has been used to structure the complex information processing for real-time sensory interactive robot control in a manageable form. This structure consists of a number of generic control levels. The task of a generic control level is to sample its input state and generate an appropriate response output state which results in a partial decomposition of its task command. Sensory feedback is provided by a processing structure of modules that are coupled with the appropriate control levels. The requirement that the system must be designed for ease of human comprehension has led to an implementation using a state-table processing structure. Real-time response results from a multiple processor implementation using synchronized communications through a common memory.

501,072
PB85-202570 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Kinematic Equations for Industrial Manipulators.
Final rept.,
D. R. Myers, and D. F. Gordon. 1982, 4p
Pub. in Ind. Robot. 9, n3 p162-165 Sep 82.

Keywords: *Robots, Equations of motion, Kinematics, Manipulators, Automation, Control, Reprints, Computer applications.

A method is presented for developing the kinematic equations of motion for a six degree-of-freedom manipulator in a manner which can be generalized for ap-

plication to most commercially available robots. In using this method, Cartesian coordinate frames are assigned to each link such that the number of transcendental and arithmetic operations needed to transform from coordinates in one frame to those in any other frame is minimized. Also presented is a method to solve the kinematic equations for each of the joint angles.

501,073
PB86-102365 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Industrial Systems Div.
Adjustment of Robot Joint Gears Using Encoder Velocity and Position Information.
Final rept.,
N. G. Dagalakis, and D. R. Myers. 1985, 6p
Pub. in International Jnl. of Robotic Systems 2, n2 p229-234, 1985.

Keywords: *Robots, Gears, Setting(Adjusting), Algorithms, Linkages, Systems engineering, Reprints.

A new technique for the adjustment of joint gears in industrial robots is presented. Band-limited random excitation signals were injected into the drive system of the joint under test, and both the actuator shaft velocity and position were monitored. The coherence functions between the voltage at the terminals of the electric actuator and the position and velocity signals were determined. The change in the coherence functions was studied for various joint gear settings. An algorithm is proposed for determining the gear setting which results in the most linear operation of the joint drive system. This algorithm was tested on the adjustment of the gears of the wrist rotation joint of a PUMA 560 robot arm.

501,074
PB86-102373 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Industrial Systems Div.
Adjustment of Robot Joint Gear Backlash Using the Robot Joint Test Excitation Technique.
Final rept.,
N. G. Dagalakis, and D. R. Myers. 1985, 15p
Contract N00014-83-K-0236
Sponsored by Office of Naval Research, Arlington, VA.
Pub. in International Jnl. Robotics Research 4, n2 p65-79, 1985.

Keywords: *Robots, *Gears, Joints(Junctions), Adjusting, Backlash, Reprints, *Robotics, System identification.

A technique has been developed for the precise adjustment of gear backlash of the joints of an industrial robot. Band limited random excitation signals were injected into the drive system of the joint under test, and the output response of the joint link was monitored using an accelerometer. The coherence function was measured and used to adjust the joint gear backlash in order to minimize the effect of the backlash nonlinearity on the joint drive system. Tests were performed while the joint was both loaded and unloaded and for several different steady state positions. The test results indicate that this technique can be used for both the adjustment of the joint gears and the periodic automatic inspection of their condition.

501,075
PB86-103637 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Industrial Systems Div.
Robotics.
Final rept.,
J. S. Albus. 1984, 29p
Sponsored by Department of the Army, Washington, DC.
Pub. in NATO Advanced Study Institute Series F11, p65-93 1984.

Keywords: *Robots, Visual perception, Reprints, *Robotics, Hierarchical control, Knowledge representation.

Major problems areas in robotics are enumerated: 1. Kinematics, dynamics, and mobility; 2. Sensors and Sensory Processing; 3. Control; 4. Knowledge Representation and Modeling; 5. Programming Methodology; 6. Interfaces and Communications. A hierarchical robot control architecture is described which partitions the task decomposition into eight levels; four in the robot (1) servo and coordinate transformation, (2) elemental movement, (3) simple task, (4) complex task;

Field 13—MECHANICAL, INDUSTRIAL, CIVIL, AND MARINE ENGINEERING

Group 13I—Machinery and Tools

and four in the automatic factory, (5) task sequencing (work station), (6) part batch routing (cell), (7) long range scheduling (shop), (8) process planning, product design, and management coordination (factory). This model is used to tie together the dynamic interaction between control, sensory processing, modeling, and planning. A network architecture for robots in a small automated machine shop is used to illustrate the interface and communications issues.

501,076
PB86-123007 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Industrial Systems Div.
Visual Feedback for Robot Control.
Final rept.,
M. Shneider, S. Nagalia, J. Albus, and R. Haar. 1982, 5p
Sponsored by Institute of Electrical and Electronics Engineers, Inc., New York.
Pub. in Proceedings of 1982 Workshop Industrial Applications of Machine Vision, Research Triangle Park, NC., May 3-5, 1982, p232-236.

Keywords: *Robots, *Feedback control, Visual perception, Positioning, Rangefinding, Sensory perception.

The roles of three kinds of visual information in robot control are discussed. Range information, obtained from a plane-of-light triangulation system is used in conjunction with floodlighting to find the three dimensional positions and orientations of parts and to calculate their shape properties. Information obtained from successive frames is used in a simple manner to provide feedback in approaching and acquiring a part. The three kinds of information, acting together, provide for fast and reliable object acquisition.

501,077
PB86-123148 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Automated Production Technology Div.
Design and Testing of a Fast Tool Servo for Diamond Turning.
Final rept.,
S. R. Patterson, and E. B. Magrab. 1985, 6p
Sponsored by Defense Advanced Research Projects Agency, Arlington, VA.
Pub. in Precision Engineering 7, n3 p123-128 Jul 85.

Keywords: *Diamonds, *Tools, *Servomechanism, Accuracy, Resolution, Reprints.

A self-contained and independently servo-operated diamond tool holder was built to increase the resolution and accuracy of a precision lathe. Its static and dynamic repeatability over a range of plus or minus 50 micrometers (1.27 micrometer) is better than 0.05 micrometer (1.3 micrometer). Its frequency distortion from 0-100 Hz is less than 1.0 micrometer (25 micrometer) for a peak displacement of less than 28 micrometer (0.71 micrometer).

13J. Marine Engineering

501,078
PB85-184745 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Chemical Waste Incinerator Ships: The Interagency Program to Develop a Capability in the United States.
Final rept.,
G. O. Chapman, D. W. Leubecker, L. A. Martinez, R. T. Matthews, and D. A. Oberacker. 1982, 16p
Sponsored by Society of Naval Architects and Marine Engineers, New York.
Pub. in Marine Technology 19, n4 p325-340 Oct 82.

Keywords: *Incinerators, *Ships, *Solid waste disposal, *Hazardous materials, Regulations, Design, Construction, Safety, Operations, Environmental impacts, Air pollution, Substitutes, Reprints, *Liquid waste disposal, *Chemical wastes, Waste management.

In February 1980, an interagency work group undertook a study of at-sea incineration and the alternatives available to the Federal Government for encouraging the design, construction, and operation of U.S.-flag incinerator ships. The group examined previous incineration operations, various federal assistance programs,

safety and control measures, incinerator ship conceptual designs, environmental impacts, and waterfront facilities. This paper presents the findings of the work group and the work program which the Interagency Review Board has initiated. Important ship design factors, such as the regulatory requirements, incinerator technologies, and incinerator system research recommendations, are explained. Details of a conceptual dual-mission ship design, that can incinerate both liquid wastes and solid wastes, are given. Anticipated operating permits, environmental monitoring, and waterfront facilities are discussed.

501,079
PB86-103488 PC A05/MF A01
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.
Fire Growth in Combat Ships.
J. G. Quintiere, H. R. Baum, and J. R. Lawson. Jun 85, 100p NBSIR-85/3159
Sponsored by David. W. Taylor Naval Ship Research and Development Center, Bethesda, MD.

Keywords: *Fires, *Combatant ships, Explosions, Computation, Fire damage, Mathematical models, Flame propagation, *Ship fires, *Fire growth.

A discussion of fire phenomenology pertaining to ships is presented. It draws on background from ship fires, combat ship construction characteristics and scientific knowledge developed for building fires. Its immediate goal is to assess the prospect of developing a deterministic (physics) model for ship fire growth as initiated by explosive weapon effects. A specific analysis of vented explosion flows is given as well as a procedure for computing fire growth phenomena from formulae.

501,080
PB86-130226 PC A04/MF A01
National Bureau of Standards, Gaithersburg, MD.
Response of Complaint Offshore Platforms to Waves.
M. Grigoriu, and B. Alibe. Sep 85, 61p NBS/GCR-85/501
Prepared in cooperation with Cornell Univ., Ithaca, NY. School of Civil and Environmental Engineering. Sponsored by Minerals Management Service, Reston, VA.

Keywords: *Ocean waves, *Offshore structures, Stabilized platforms, Response, Mathematical models, Monte Carlo method, Random processes.

Probabilistic descriptors are developed for the response of structures of the Tension Leg Platform type to current and waves. These are obtained by Monte Carlo techniques by assuming the validity of the Morison equation. The results are compared to those obtained by using statistical linearization techniques. Also, for offshore platforms with higher natural periods of vibration, mean upcrossing rates for various levels of the structural response are estimated by simulation, by statistical linearization techniques, and by additional procedures developed in the report.

13K. Pumps, Filters, Pipes, Fittings, Tubing and Valves

501,081
PATENT-4 494 563 Not available NTIS
Department of the Army, Washington, DC.
Fluid Safety Valve.
Patent,
J. F. N. Seiler. Filed 12 Nov 82, patented 22 Jan 85, 4p PB86-174539, PAT-APPL-6-441 311
This Government-owned invention available for U.S. licensing and, possibly, for foreign licensing. Copy of patent available Commissioner of Patents, Washington, DC 20231 \$1.00.

Keywords: *Valves, *Patents, Safety devices, Instruments, Pressure control, PAT-CL-137-496.

A typical embodiment of the invention provides a means for protecting delicate instruments from damage. A flexible membrane separates two chambers in which, during ordinary operation, the fluid pressures are the same. One of the two chambers also serves as a fluid conduit in the system. Pressure loss in the system causes the higher pressure chamber to flex the membrane which closes a port in the fluid conduit chamber, thereby preventing further system pressure

loss and consequent equipment damage. The membrane, moreover, can have a small bleed to permit gradual, dampened fluid pressure release.

501,082
PB85-177962 PC A04/MF A01
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Building Technology.
Preliminary Study of the Vertical Stack to Horizontal Drain Entry Condition as an Extension to the Modeling of Unsteady Partially Filled Pipe Flow.
J. A. Swaffield, and L. S. Galowin. Feb 85, 54p NBSIR-85/3108
Prepared in cooperation with Brunel Univ., Uxbridge (England).

Keywords: *Plumbing, *Drains, *Pipe flow, Design, Pipes(Tubes), Drainage, Vents, Mathematical models, Finite difference theory, Graphs(Charts), Discharge, Buildings.

The finite difference based method of characteristics model for unsteady partially filled pipe flow was extended to include the stack to horizontal drain entry boundary condition. The conditions at drain entry are defined in terms of the energy of the terminal annular flow velocity in the stack, together with an appropriate loss coefficient as the entry function. The hydraulic solutions link the branch drains, fittings, vertical soil stack and building drain. The analysis permits any combination of drainage load patterns from simultaneous, overlapping or sequence of discharge events. Preliminary simulations utilizing this model indicates that the modeling technique extends the existing horizontal network analysis program to a simulation of multistory building drainage systems. The sizing procedure determines the hydraulic capacity of drains for specified pipe sizes, pipe pitch and well roughness factors.

501,083
PB86-138633 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Chemical Process Metrology Div.
Estimating Diverter Valve Corrections.
Final rept.,
F. E. Jones. 1984, 4p
Pub. in International Jnl. of Heat and Fluid Flow 5, n4 p247-250 Dec 84.

Keywords: *Valves, *Estimating, *Correction, Diverters, Mass flow, Gravimetric analysis, Liquid flow, Measurement, Reprints.

A new method has been developed for estimating the corrections to be made to the measured time interval for diverter valves used in primary liquid flow measurement facilities. The model relates the mass flowrate, m , to the measured mass of liquid collected and the effective collection time.

13L. Safety Engineering

501,084
PB85-150555 CP T05
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.
FAST: A Model for the Transport of Fire, Smoke and Toxic Gases.
Model-Simulation,
W. W. Jones. Sep 84, mag tape NBSIR-84/2934, NBS/DF-85/004
Source tape is in the ASCII character set. This restricts preparation to 9 track, one-half inch tape only. Identify recording mode by specifying density only. Call NTIS Computer Products if you have questions. Price includes documentation, PB85-109130.

Keywords: *Fires, *Models simulation, Fortran, Smoke, Gases, Structures, Transport properties, Mathematical models, Magnetic tapes, Toxic hazards, Compartment fires.

A numerical implementation of a zone model which will transport fire, smoke and toxic gases in a multi-compartment structure. The model includes the calculations necessary for a toxic hazard evaluation of materials. Software Description: The model is written in the FORTRAN programming language for implementation on a PERKIN-ELMER 3200 computer using the OS32/6.2 operating system. Memory requirement is 128 K bytes.

501,085
PB85-177913 PC A06/MF A01
 National Bureau of Standards, Gaithersburg, MD.
Development of a Fire Evaluation System for Detention and Correctional Occupancies,
 H. E. Nelson, and A. J. Shibe. Dec 84, 123p NBSIR-84/2976
 Sponsored by Department of Justice, Washington, DC.

Keywords: *Fire safety, *Evaluation, Safety devices, Buildings, Sprinkler systems, Fire protection, Facilities, Requirements, Design, *Correctional institutions, Evacuation egress, Fire codes.

A Fire Safety Evaluation System for Detention and Correctional Occupancies has been developed. It can be used for determining if a facility has fire safety equivalent to that obtained by meeting the requirement of a given code. The system was calibrated for use with proposed chapters for detention and correctional occupancies of the Life Safety Code (1985). There are separate sets of requirements for each of four use conditions; one for zoned egress, one for zoned impeded egress, one for impeded egress, and one for contained. Within each set, there are two levels of evaluation: one for partially sprinklered and non-sprinklered buildings, and one for totally sprinklered buildings.

501,086
PB85-178077 PC A07/MF A01
 American Inst. of Architects Foundation, Washington, DC.
Fire Emergency Evacuation Simulation for Multifamily Buildings.
 Final rept.,
 D. M. Alvord. Dec 84, 132p NBS/GCR-84/483
 Grant NB82-NADA-3043

Keywords: *Apartment buildings, *Fires, *Evacuating(Transportation), Computer programs, Computerized simulation, Residential buildings, Fire safety, Egress, Emergency escape, Fire models.

This report concerns the Fire Emergency Evacuation Simulation for Multifamily Buildings, a deterministic discrete event model for emergency evacuation from living areas of multifamily buildings. It is the final report of the project. It is written in such a fashion that those individuals who wish only general understanding of the model can easily find what they require, while those persons who require a deeper understanding can find all of the information that they need. A general introduction is first to appear. Next appears a section describing background information that a user would require to knowledgeably prepare input. A detailed description of the required input format is next to be given followed by a detailed discussion of the logic behind the various sections of the model as implemented in the program. Three example simulation runs, as well as a listing of the program, also are given.

501,087
PB85-178085 PC A04/MF A01
 Rutgers - The State Univ., New Brunswick, NJ. Dept. of Mechanical, Industrial and Aerospace Engineering.
Experimental Study of Negatively Buoyant Flows Generated in Enclosure Fires,
 Y. Jaluria, and D. Goldman. Feb 85, 53p NBS/GCR-85/487
 Grant NB83-NADA-4047

Keywords: *Enclosures, *Fires, Fluid flow, Buoyancy, Penetration, Smoke, Thermal measurements, Velocity measurement, Air flow, Fire hazards, Flow rate, Compartment fires, Room fires.

An experimental investigation of the nature of the velocity and thermal fields in negatively buoyant flows generated in enclosure fires is carried out. The flow configuration considered is that of a negatively buoyant two-dimensional jet discharged adjacent to a vertical surface, as well as that discharged away from the boundaries of the region. Such flows are frequently encountered in enclosures due to the downward turning of the flow induced by the fire plume, at the corners of the ceiling. Similarly, wall flows generated in the upper stably stratified region in room fires penetrate into the cooler, lower region. In these cases, the buoyancy force is upward while the flow is downward, resulting in a negatively buoyant circumstance. An experimental system is developed to study the downward penetration of such jets in which the buoyancy force opposes the flow. The penetration distance is measured and related to the inflow conditions, particularly the temperature and velocity at the discharge location.

501,088
PB85-179729 PC A03/MF A01
 National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.
Jefferson National Memorial Historical Site Analysis of Impact of Fire Safety Features,
 H. E. Nelson. Mar 85, 41p NBSIR-84/2897
 Sponsored by National Park Service, Washington, DC.

Keywords: *Fire safety, *Museums, Buildings, Evacuation(Transportation), Sprinkler systems, Jefferson National Memorial Historical Site, Smoke detectors.

An analysis is made of the rate of the potential intrusion of hazardous environments in a museum facility as compared to the capacity of the exit system to evacuate the occupants.

501,089
PB85-187573 PC A04/MF A01
 Florida Univ., Gainesville. Dept. of Industrial and Systems Engineering.
Network Models of Building Evacuation: Development of Software System. Final Report, March 1985,
 T. M. Kisko, and R. L. Francis. Mar 85, 60p NBS/GCR-85/489
 Grant NB81-NADA-2057
 See also PB84-217520.

Keywords: *Buildings, *Evacuating(Transportation), Fire safety, Networks, Mathematical models, EVACNET computer program, Computer applications, Means of egress.

This report summarizes the efforts of the third and final year of a project to develop EVACNET+, a user friendly computer program that models building evacuations. When the evacuation of a building involves the flow of people through well defined passageways, it is natural to consider the evacuation problem to be a network flow problem. EVACNET+ is a user friendly interactive computer program that accepts a user defined network model of a building, converts that model to a time expanded dynamic 'transshipment' network, and solves the dynamic network problem using a capacitated minimum cost network flow algorithm. The solution obtained gives a time-dependent plan to evacuate the building in a minimum time, and identifies building evacuation bottlenecks. In the first year of the grant, EVACNET+ was developed to the point of preliminary testing. During the second year, the coding of EVACNET+ was completed and a user's manual was written. This final year of the grant concentrated on research related to extensions of the EVACNET+ concept. Areas of research included investigating: Time-varying extensions of EVACNET+; A model controlled adjustment option; Integration of EVACNET+ with other models; New solution procedures for EVACNET+; Expanded model input and editing functions; A result data base analysis system. A microcomputer version of EVACNET+ was also developed for the IBM PC or equivalent.

501,090
PB85-187581 PC A03/MF A01
 National Bureau of Standards (NEL), Gaithersburg, MD.
Literature Survey on Drop Size Data, Measuring Equipment and Discussion of the Significance of Drop Size in Fire Extinguishment,
 W. D. Hayes. Jan 85, 31p NBSIR-85/3100
 Sponsored by Federal Emergency Management Agency, Washington, DC.

Keywords: *Drops(Liquids), *Fire extinguishing agents, Size determination, Measuring instruments, Spraying, Water, Nozzles, Fire fighting.

The literature was searched for information and data on the size of water droplets from fire fighting equipment, on instrumentation and techniques for measuring droplet size in dense sprays, and on the significance of droplet size in water sprays used for fire extinguishment. Included is a discussion of droplet size information on an impinging jet type fire hose nozzle. Droplet size analyzers that use shadowgraphic technique are likely to be best suited for measuring sprays from fire hose nozzles. The effects of droplet size in water sprays used for extinguishment in confined and unconfined spaces and with and without counterflowing air currents is discussed.

501,091
PB85-196616

(Order as PB85-196541, PC A07/MF A01)
 Underwriters' Labs., Inc., Northbrook, IL.

Survey of the State of the Art of Mathematical Fire Modeling,
 J. S. Parikh, and J. R. Beyreis. Apr 85, 19p
 Sponsored by National Bureau of Standards (NEL), Gaithersburg, MD. Center for Building Technology, and National Conference of States on Building Codes and Standards, Inc., Herndon, VA.
 Included in Research and Innovation in the Building Regulatory Process: Proceedings of the NBS/NCSBCS Joint Conference (6th), Technical Seminar on Streamlined Administrative Procedures, Computers in Construction, and Fire Safety Technology held at Denver, Colorado on September 11, 1984, p93-111 Apr 85.

Keywords: Fires, Mathematical models, Surveys, Flame propagation, Design, *Fire models.

In the past decade, considerable effort and resources have been directed at the development and use of mathematical modeling for predicting the fire response of products in a particular fire situation. Recently, Underwriters Laboratories Inc. (UL) undertook a survey of the state of the art of mathematical fire modeling for predicting the growth of a fire within a room under the sponsorship of the Society of the Plastics Industry. The objective was to assist in bridging the application of mathematical fire modeling from fire researcher to fire practitioner.

501,092
PB85-196632

(Order as PB85-196541, PC A07/MF A01)
 Travelers Insurance Co., Hartford, CT.
Non-Evacuation in Compartmented Fire Resistive Buildings Can Save Lives and It Makes Sense,
 J. N. Macdonald. Apr 85, 14p
 Sponsored by National Bureau of Standards (NEL), Gaithersburg, MD. Center for Building Technology, and National Conference of States on Building Codes and Standards, Inc., Herndon, VA.
 Included in Research and Innovation in the Building Regulatory Process: Proceedings of the NBS/NCSBCS Joint Conference (6th), Technical Seminar on Streamlined Administrative Procedures, Computers in Construction, and Fire Safety Technology held at Denver, Colorado on September 11, 1984, p117-130 Apr 85.

Keywords: *Fire resistance, *Buildings, Fire safety, Fires, *Evacuation, *Compartmentalization.

Compartmented fire resistive buildings are used for hotels, motels, apartments, condominiums, dormitories, hospitals, and other health care facilities. Several fires in compartmented fire resistive buildings were reviewed. Not all of those that were reviewed were used in this study, only those where reasonably accurate conclusions could be drawn as to whether the victims had evacuated or not.

501,093
PB85-196640

(Order as PB85-196541, PC A07/MF A01)
 Totel Systems, Inc., Stratford, CT.
Telephone Connected Early Warning and Communication System,
 W. M. Smith. Apr 85, 5p
 Sponsored by National Bureau of Standards (NEL), Gaithersburg, MD. Center for Building Technology, and National Conference of States on Building Codes and Standards, Inc., Herndon, VA.
 Included in Research and Innovation in the Building Regulatory Process: Proceedings of the NBS/NCSBCS Joint Conference (6th), Technical Seminar on Streamlined Administrative Procedures, Computers in Construction, and Fire Safety Technology held at Denver, Colorado on September 11, 1984, p131-135 Apr 85.

Keywords: *Warning systems, *Telephone equipment, *Communication equipment, Buildings, Fire fighting, Fire safety, Smoke detectors.

This paper describes a new development in telephone engineering that provides two vital fire fighting functions - annunciation of smoke detectors by individual location, and one way voice communication to remote sections of buildings by zone or all-call using existing standard telephone equipment. This development creates an opportunity for advanced fire systems features to be put in place quickly and at low cost since most structures already have complete telephone system

Field 13—MECHANICAL, INDUSTRIAL, CIVIL, AND MARINE ENGINEERING

Group 13L—Safety Engineering

wiring and standard station line telephones throughout the building.

501,094
PB85-198935 PC A03/MF A01
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.
ASET-B, a Room Fire Program for Personal Computers,
W. D. Walton. Apr 85, 41p NBSIR-85/3144
Sponsored by National Park Service, Washington, DC. and Department of Health and Human Services, Washington, DC.

Keywords: *Fires, Flame propagation, Manuals, Evacuating(Transportation), BASIC(Programming language), Computer programs, Smoke, ASET-B computer program, Room fires, Compartment fires.

ASET-B, a personal computer program for predicting the fire environment in a single room, is presented. ASET-B solves the same differential equations as the previously developed computer program, ASET (Available Safe Egress Time), using a simpler numerical technique. ASET-B requires as input the height and area of the room, the elevation of the fire above the floor, a heat loss factor, and a fire specified in terms of heat release rate. The program predicts the thickness and the temperature of the hot smoke layer as a function of time. ASET-B is written in BASIC and is not subject to copyright. This paper describes the program and its use. Included are a listing of the program, program variable name listing and a sample run. A discussion of user modifications also is given.

501,095
PB85-199545 PC A99/MF A01
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.
Proceedings of the Joint Panel Meeting of the UJNR Panel on Fire Research and Safety (7th) Held at Gaithersburg, Maryland on October 24-28, 1983,
N. H. Jason, and K. Davis. Mar 85, 652p NBSIR-85/3118
See also N84-13341.

Keywords: *Meetings, *Fire safety, Risk, Measurement, Combustion, Flame propagation, Toxicity, Buildings, Construction materials, Hazards, Tests, Materials, *Fire research.

The 7th Joint Panel Meeting of the United States-Japan Panel on Fire Research and Safety was held jointly with the Combustion Toxicity and 2nd Expert Meeting of the U.S.-Japan-Canada Cooperative Research Group on Toxicity of Combustion Products from Building Materials and Interior Goods at the National Bureau of Standards, Gaithersburg, Maryland, October 24-28, 1983. Technical sessions were in the areas of: Fire Hazard/Risk Management Methods; Fire Growth Prediction; Materials Fire Properties and Test Methods; Measurement Methods; Combustion Toxicity. Progress reports were presented in each area, in addition to state-of-the-art papers. The next conference will be held in Japan in May 1985.

501,096
PB85-200103 PC A03/MF A01
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.
Buoyant Plume-Driven Adiabatic Ceiling Temperature Revisited,
L. Y. Cooper, and A. Woodhouse. Apr 85, 32p NBSIR-85/3134

Keywords: *Heat transfer, *Convection, *Fires, *Buildings, Coillings(Architecture), Plumes, Mathematical models, Walls, Adiabatic conditions, Temperature distribution, Research.

In previous works, the convective heat transfer from buoyant plume-driven ceiling jets to unconfined ceilings has been estimated using a formula for the temperature distribution below an adiabatic ceiling. Tad, obtained from experimental data. The present study re-evaluates this data, and develops an independent estimate for Tad. The analysis takes account of the effect of ceiling surface re-radiation, and use is made of the previously established similarity between plume/ceiling- and jet/wall-driven heat transfer phenomena. The latter similarity is the basis of a correlation of recently reported free jet-wall jet 'recovery temperature' data into a normalized Tad distribution. All of the analysis leads to new formulae for estimating the convective heat transfer to ceilings during enclosure fires.

501,097
PB85-202786 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Fire Safety Technology Div.
Emerging Engineering Methods Applied to Fire Safety Design.
Final rept.,
H. E. Nelson. 1985, 4p
Pub. in Proceedings of Research and Design 1985: Architectural Applications of Design and Technology Research at Los Angeles, CA., on March 14-18, 1985, p181-184.

Keywords: *Fire safety, Buildings, Design, Building codes, Fire protection, Tests, Safety engineering.

The development of fire science has progressed to a point where an analytical engineering methodology for fire protection design is emerging. This presentation outlines the elements of such a method and provides an example of one facet and a broad range of references for those interested in deeper examination.

501,098
PB85-203479 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Analysis of Smoldering Fires in Closed Compartments and Their Hazard Due to Carbon Monoxide.
Final rept.,
J. G. Quintiere, M. M. Birky, F. Macdonald, and G. Smith. 1982, 2p
See also PB82-257684.
Pub. in Fire and Materials 6, n3-4, p99-110 Sep-Dec 82.

Keywords: *Buildings, *Fire hazards, *Carbon monoxide, Fire tests, Lethal dosage, Mathematical models, Risk, Reprints, *Room fires, *Smoldering fires, Computer applications.

A review was made of smoldering fire experiments conducted in closed rooms and buildings. The results were summarized by tabulating maximum levels of CO, the time integral of CO concentration ('dose'), CO₂, temperature rise and oxygen consumption. A hazard time based on the attainment of a CO dose equal to 4.5% CO-minutes and the time for transition to flaming were also tabulated. The chance of reaching a critical CO condition during smoldering seems to be comparable to the chance of having transition to flaming occur. A theoretical model, requiring inputs of CO production rate and energy release rate, was executed and compared with available data. The theoretical results for CO concentration as a function of time were in good agreement with the experimental data. The model offers a means of extrapolating test data to compartments of various size in order to assess the general hazard of CO due to smoldering.

501,099
PB85-208015 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Fire Safety Technology Div.
Design as a Function of Responses to Fire Cues.
Final rept.,
B. M. Levin. 1985, 6p
Pub. in Proceedings of Research and Design '85: Architectural Applications of Design and Technology Research, Los Angeles, CA., March 14-18, 1985, p289-294.

Keywords: *Buildings, *Design, *Fire safety, *Human behavior, Safety engineering, Architecture, Evacuation, Means of egress.

Studies of the actions of building occupants in fire emergencies show that people often do not initiate an evacuation immediately upon hearing an alarm or smelling smoke. Unless the size, location and danger of the fire is obvious, investigation is a likely action. In addition, ignoring the first signs of a fire is not a rare event. Once an evacuation is initiated, people often attempt to leave by the most familiar rather than most direct route and they often do not or cannot see and follow exit signs. The paper provides current state of the art guidance on how people respond in fire emergencies and how the architect can modify total designs (including alarms, public address systems, location of and approaches to emergency exits, etc.) to take advantage of the anticipated response of the occupants in danger. The information will aid the architect in developing designs that increase the likelihood that building occupants will use the emergency evacuation system as the architect intended.

501,100
PB85-208023 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Fire Measurement and Research Div.
Calculations of the Heat Release Rate by Oxygen Consumption for Various Applications, September-October 1984.
Final rept.,
W. J. Parker. Oct 84, 6p
See also PB82-192956.
Pub. in Jnl. of Fire Sciences 2, n5 p380-395 Sep/Oct 84.

Keywords: *Fire tests, *Heat measurement, Computation, Calorimeters, Oxygen consumption, Formulas(Mathematics), Reprints, *Heat release rate, Room fires.

The calculation of heat release rate by oxygen consumption is based on the assumption that all materials release approximately the same amount of heat per unit mass of oxygen consumed. The technique is now being employed to determine the heat release rate of materials in various heat release rate calorimeters. Other uses include the heat release rate of assemblies in the fire endurance furnaces and the total heat release rate in room fire tests. Various assumptions about CO levels in the exhaust duct and vitiation and humidity in the incoming air are made. General formulas for the heat release rate by oxygen consumption are developed in the paper from which the formulas for specific applications can easily be derived.

501,101
PB85-229946 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Operations Research Div.
Economics of Fast-Response Residential Sprinkler Systems.
Final rept.,
R. T. Ruegg, and S. K. Fuller. 1985, 10p
Pub. in Fire Jnl. 79, n3 p18-22/115-118 May 85.

Keywords: *Sprinkler systems, *Fire protection, Economic analysis, Decision making, Reprints, *Residential buildings, Life-cycle cost, Risk analysis, Benefits.

The article presents in brief, illustrates and discusses a model for assessing the economic feasibility of fast-response sprinkler systems for houses. The model calculates expected net present value benefits as they would accrue to the owner of a system, as well as break-even values for key decision variables. Nine hypothetical cases are based on the application of a specified system in a new, single-family dwelling, 'average' levels of fire risk as indicated by recent aggregate U.S. fire loss statistics, and sprinkler system performance based on the results of laboratory and field tests of system effectiveness. The results have implications of interest to the research and building communities concerned with the economics of home fire protection.

501,102
PB85-234946 PC A03/MF A01
National Bureau of Standards (NEL), Boulder, CO.
Literature Survey on Drop Size Data, Measuring Equipment, and a Discussion of the Significance of Drop Size in Fire Extinguishment,
W. D. Hayes. Jul 85, 31p NBSIR-85/3100/1
Sponsored by Federal Emergency Management Agency, Washington, DC.

Keywords: *Fire extinguishing agents, *Drops(Liquids), Fire extinguishers, Fire fighting, Spraying, Water, Measurement, Fire hoses, Spray nozzles.

The literature was searched for information on the size of water droplets from fire fighting equipment, on instrumentation and techniques for measuring droplet size in dense sprays, and on the significance of droplet size in water sprays used for fire extinguishment. From the information on drop size analyzers gathered, it is likely that analyzers using a shadowgraphic method to measure drop size are best suited for drop size measurements in water sprays from fire hose nozzles. The effects of droplet size in water sprays used for extinguishment is confined and unconfined spaces and with and without counterflowing air currents are discussed. The report supersedes the January 1985 edition (NBSIR 85-3100).

501,103
PB85-236370 PC A11/MF A01
 American Inst. of Architects Foundation, Washington, DC.
Status Report on the Escape and Rescue Model and the Fire Emergency Evacuation Simulation for Multifamily Buildings,
 D. M. Alvord. Jun 85, 233p NBS/GCR-85/496
 Contract NB82-NADA-3043

Keywords: *Fire safety, *Residential buildings, Computer programs, Computerized simulation, Rescue operations, *Building fires, *Emergency escape, *Health care facilities, Life safety, Evacuation, Means of egress, Group homes.

The report concerns changes made to the Escape and Rescue Model and the Fire Emergency Evacuation Simulation for Multifamily Buildings to enhance their portability and user-friendliness. Both model programs were changed from SIMSCRIPT II.5 to Fortran and were revised in order to permit interactive access. The report consists of a brief overview of the Escape and Rescue Model as well as an overview of the other model. Next appears a chapter detailing the changes performed to the model programs. User's guides to running the programs implementing each model are next to appear in the form of appendices. Finally, example computer runs and listings of each program are given.

501,104
PB85-240901 PC A04/MF A01
 National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.
Jet Diffusion Flame Suppression Using Water Sprays, Final Report,
 B. J. McCaffrey. Jul 85, 58p NBSIR-84/2812-1
 Supersedes PB84-159052. Sponsored by Minerals Management Service, Washington, DC.

Keywords: *Offshore drilling, *Fire protection, *Blow-outs, Water, Spraying, Gas wells, Oil wells, Fire extinguishing agents, Nozzles, Thermodynamic equilibrium, Diffusion flames, Temperature, Fires, Retarding, Water spray.

The feasibility of using water sprays for the control of offshore oil/gas well blowout fires has been addressed. Considering the sheer scale of the problem, knowledge from a fundamental viewpoint is going to be required in order to extrapolate laboratory-sized flame studies up to full scale. Available data and appropriate literature concerned with the application of water sprays as a jet diffusion flame suppression/extinguishment agent have been reviewed. Small pneumatic atomizing nozzles using H₂ gas, both as the flame source as well as the atomizing driver, have been used to scale high momentum jet flames and to study the effect of water on the flame. Thermodynamic equilibrium was shown to be an effective guide in interpreting the results. The effect of flame temperature reduction due to water sprays has been observed to correlate with a single spray parameter - the median drop diameter.

501,105
PB86-101029 PC A03/MF A01
 National Bureau of Standards (NEL), Washington, DC. Center for Applied Mathematics.
Applied Model Validation,
 A. D. Davies. Jul 85, 32p NBSIR-85/3154/1

Keywords: *Fires, *Smoke, Temperature, Computation, *Fire models, *Toxic gases, Fire spread, Fire tests, Computer applications.

The progress report is about an applied model validation case study. The subject model is 'Transport of Fire, Smoke and Toxic Gases (FAST)' by W. W. Jones of the National Bureau of Standards, Center for Fire Research. Products from a fire in a 'burn room' exit through a connected corridor to outdoors. Cooler counterflow air in a lower layer feeds the fire. The model predicts corridor layer temperatures and thicknesses vs. time, given enclosure, fire and ambient specifications. Data have been collected from 38 tests using several fire sizes, but have not been reduced. Corresponding model results, and model and test documentation are yet to come. Considerable modeling and calculation is needed to convert instrument readings to test results comparable with model outputs so that residual differences may be determined. Test results as well as model results must be validated, and test result uncertainties estimated so that they are not unfairly attributed to the model.

501,106
PB86-105970 PC A03/MF A01
 National Bureau of Standards (NEL), Gaithersburg, MD.
Application of Models to the Assessment of Fire Hazard from Consumer Products.
 Final rept.,
 R. W. Bukowski. Aug 85, 32p NBSIR-85/3219
 Sponsored by Consumer Product Safety Commission, Washington, DC.

Keywords: *Fire hazard, Mathematical models, Evaluation, Risk, Furniture, Bedding equipment, Toxicity, Combustion.

The differences among models of fire, fire hazard, and fire risk are described. The use of field, zone, and network models for fire hazard assessment is discussed. A number of available single and multiple compartment models are described. Key considerations with respect to the use of the current models by the Consumer Product Safety Commission for hazard assessment from upholstered furniture and mattress fires is presented. Modifications necessary to improve the capability of these models for hazard assessment are identified. Model validation, output presentation, and data sources are discussed. Recommendations on specific models for the sponsor to consider for further study and use are provided.

501,107
PB86-105996 PC A03/MF A01
 National Bureau of Standards (NEL), Gaithersburg, MD.
Methods to Calculate the Response Time of Heat and Smoke Detectors Installed Below Large Unobstructed Ceilings,
 D. D. Evans, and D. W. Stroup. Jul 85, 50p NBSIR-85/3167
 Sponsored by Nuclear Regulatory Commission, Washington, DC.

Keywords: *Early warning systems, Safety devices, Computer programs, Heat measurement, Heat transmission, Detection, Reaction time, Feedback control, Fortran, *Smoke detectors.

Recently developed methods to calculate the time required for ceiling mounted heat and smoke detectors to respond to growing fires are reviewed. A computer program, that calculates activation times for both fixed temperatures and rate of rise heat detectors in response to fires that increase in heat release rate proportionally with the square of time from ignition, is given. This program produces equivalent results to the tables published in Appendix C, Guide for Automatic Fire Detector Spacing, (NFPA 72E, 1984). A separate method and corresponding program are provided to calculate response time for fires having arbitrary heat release rate histories. This method is based on quasi-steady ceiling layer gas flow assumptions. Assuming a constant proportionality between smoke and heat release from burning materials, a method is described to calculate smoke detector response time modeling the smoke detector as a low temperature heat detector in either of the two response time models.

501,108
PB86-106002 PC A08/MF A01
 National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.
Fire Performance of Interstitial Space Construction Systems,
 J. R. Lawson. May 85, 165p NBSIR-85/3158
 Errata sheet inserted. Sponsored by Veterans Administration, Washington, DC.

Keywords: *Fire tests, Steel structures, Fire resistance, Tests, Graphs(Charts), Structural members.

Two unique walk-on deck construction systems were exposed to the standard NFPA 251 time-temperature fire exposure for periods up to two hours in order to evaluate their fire performance. A large scale steel structure was used in the test program to simulate construction systems found in the field. The structure consisted of two large functional floors separated by an interstitial space in which a walk-on deck was suspended from the top functional floor. One of the walk-on deck systems was constructed from lightweight concrete, and the second was built with poured gypsum. Critical components evaluated were the top functional floor, unprotected steel work in the interstitial space, the walk-on deck system, and protection for a heavy steel column located in the center of each test

bay. Test data were compared with the fire endurance test requirements of NFPA 251. Computer predictions also were made using the FIRES-T3 model to determine its ability to accurately predict the construction systems performance.

501,109
PB86-122876 Not available NTIS
 National Bureau of Standards (NEL), Gaithersburg, MD. Fire Safety Technology Div.
Harvard Fire Model.
 Final rept.,
 H. E. Miller. 1985, 10p
 Pub. in Fire Safety Jnl. 9, p7-16 1985.

Keywords: *Fire tests, Fire safety, Mathematical models, Reprints, *Fire models, Computer applications.

The paper gives an overview of the Harvard Computer Fire Code. Some background on mathematical fire modeling in general is given and then some of the assumptions and approximations made in the Harvard Mark 5 model are outlined. The capabilities of the model are then discussed, as well as the two variants, Mark 5.3 and Mark 6. The validity and reliability of the model are considered, and its weakest features noted. The requirements in terms of machine size, CPU time, and data are considered, as well as the input/output for (from) the program. Finally, how the program can be modified, plus plans for its future development, are outlined.

501,110
PB86-130986 PC A03/MF A01
 National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.
Data Sources for Parameters Used in Predictive Modeling of Fire Growth and Smoke Spread,
 D. Gross. Sep 85, 41p NBSIR-85/3223

Keywords: *Flame propagation, *Flammability testing, Fire point, Burning rate, Combustion products, Smoke, Thermophysical properties.

Sources of data needed for predictive modeling of fire growth by FAST and ASET, two computer codes developed at the Center for Fire Research, are identified for a few selected materials. Data includes thermophysical properties of compartment lining materials and burning rates and combustion product generation rates for typical combustible contents.

501,111
PB86-136603 PC A03/MF A01
 National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.
Comparison of Several Compartment Fire Models: An Interim Report,
 H. E. Miller. Oct 85, 37p NBSIR-85/3233
 Sponsored by Nuclear Regulatory Commission, Washington, DC.

Keywords: *Fire tests, Compartment analysis, Comparison, Mathematical models, Fire walls, Fire hazards, *Fire models.

A substantial number of mathematical models for compartment fires have been developed in the past decade. The report analyzes and compares in depth three such models. This is done with particular emphasis on the needs of the Nuclear Regulatory Commission and Sandia National Lab, for their Risk Methods Integration and Evaluation Program. The models examined are: (1) the Harvard family of models, Mark 5, 5.2, 5.3, and 6; (2) COMPBRN; and (3) FAST.

501,112
PB86-138625 Not available NTIS
 National Bureau of Standards (NEL), Gaithersburg, MD. Fire Safety Technology Div.
Multicompartment Model for the Spread of Fire, Smoke and Toxic Gases.
 Final rept.,
 W. W. Jones. 1985, 25p
 Pub. in Fire Safety Jnl. 9, p55-79 1985.

Keywords: Fire tests, Mathematical models, Smoke, Toxicity, Reprints, *Fire models.

A numerical implementation of a zone model which will transport fire, smoke and toxic gases in a multi-compartment structure is described. The areas covered are the equations which are solved, the numerical technique for the solution of these equations, species

Field 13—MECHANICAL, INDUSTRIAL, CIVIL, AND MARINE ENGINEERING

Group 13L—Safety Engineering

transport and the other relevant physical phenomena which govern fire growth and spread, and the transport of smoke. Also included in the model are the calculations necessary for a toxic hazard evaluation of a structure with a specific material loading.

501,113
PB86-139680 PC A07/MF A01
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.
Summaries of Center for Fire Research (of the National Bureau of Standards) Grants and In-House Programs - 1985.
S. M. Cherry. Nov 85, 150p NBSIR-85/3258
See also PB85-200202.

Keywords: *Fire tests, *Abstracts, Fire control, Combustion, Flame propagation, Soot, Smoke, *Fire studies, Fire models.

The report contains extended abstracts of grants and contracts for fire research sponsored by the Center for Fire Research, National Bureau of Standards, as well as descriptions of the internal programs of the Center for Fire Research.

501,114
PB86-139755 PC A04/MF A01
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.
Establishment of a Catalog of Compartment Fire Model Algorithms and Associated Computer Sub-routines.
D. W. Stroup. Nov 85, 52p NBSIR-85/3263

Keywords: *Catalogs(Publications), Algorithms, Computer programs, Mathematical models, *Compartment fires, *Fire models, Fire studies.

The Compartment Fire Model Research group of the Center for Fire Research, National Bureau of Standards has been charged with the development of a 'benchmark' compartment fire model. As part of this activity, a catalog of available fire model algorithms is being compiled. The paper presents a proposal for the organization, format, and use of the catalog.

501,115
PB86-153491 PC A03/MF A01
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.
User's Guide for FAST.
W. D. Walton, S. R. Baer, and W. W. Jones. Dec 85, 36p NBSIR-85/3284

Keywords: *Fires, Computer programs, Smoke, *Compartment fires.

FAST is a multicompartment zone type computer model which predicts the smoke hazard development in each compartment based on a description of the compartments and the fire. A FORTRAN program has been written for the model. The user's guide provides a detailed description of the data input requirements and the output produced by version 17 of the program. Also included are sample program input and output.

501,116
PB86-153913 PC A03/MF A01
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.
ASET-B: A Room Fire Program for Personal Computers.
W. D. Walton. Dec 85, 42p NBSIR-85/3144-1
Sponsored by National Park Service, Washington, DC., and Department of Health and Human Services, Washington, DC.

Keywords: *Fires, *Forecasting, Computer programs, Smoke, *Compartment fires, Fire studies.

ASET-B, a personal computer program for predicting the fire environment in a single room, is presented. ASET-B solves the same differential equations as the previously developed computer program, ASET (Available Safe Egress Time), using a simpler numerical technique. ASET-B requires as input the height and area of the room, the elevation of the fire above the floor, a heat loss factor, and a fire specified in terms of heat release rate. The program predicts the thickness and the temperature of the hot smoke layer as a function of time. ASET-B is written in BASIC and is not subject to copyright. This paper describes the program and its use. Included are a listing of the program, program variable name listing and a sample run. A discussion of user modifications also is given.

501,117
PB86-159357 PC A07/MF A01
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.
National Fire Research Strategy Conference Proceedings, July 22-25, 1985.
Final rept.,
B. M. Levin. Dec 85, 126p NBSIR-85/3290
Sponsored by National Fire Protection Association, Quincy, MA.

Keywords: *Fire safety, *Meetings, Research, Fire prevention, Fire fighting, Fire protection, Planning, Risk assessment.

The July 22-25, 1985, meeting of the National Fire Research Strategy Conference was held for the purpose of initiating the development of a coordinated fire research plan to achieve the reduction in fire losses in the United States in accord with the objectives of the Fire Prevention and Control Act of 1974. One hundred and seventeen experts from industry, government, academia, and professional societies were assigned to one of nine panels or workshops to discuss different application areas of fire research and the needed research in the respective areas. The areas included: design and engineering; materials and products; investigation and litigation; regulation and risk; real time fire extinguishment; and fire prevention, safety and survival.

501,118
PB86-166196 PC A03/MF A01
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.
Naval Fire Fighting Trainers: Effect of Ventilation on Fire Environment (Model Calculations for 19F3 FFT).
B. J. McCaffrey, J. A. Rockett, and R. S. Levine. Dec 85, 32p NBSIR-85/3238
Sponsored by Naval Training Equipment Center, Orlando, FL.

Keywords: *Entrainment, Fires, Models, Safety, Plumes, Simulation, Ventilation, *Fire models.

The Harvard 5.2 Mathematical Fire Growth Model was used to calculate required ventilation rates for two simulated fire scenarios in the Navy 19F3 trainer. These calculations were performed for design purposes to insure that the hot gas layer temperature in the trainer would be acceptable and that the oxygen content of the gas would be above 18%. Wall temperatures were also calculated.

13M. Structural Engineering

501,119
PB85-186906 PC A11/MF A01
Virginia Polytechnic Inst. and State Univ., Blacksburg. Dept. of Mechanical Engineering.
Thermal Performance Testing and Mathematically Modeling of Integral Collector Storage Solar Hot Water Systems.
Final rept.,
W. C. Thomas. Feb 85, 234p VPI-E-85-5, NBS/GCR-85/490
Grant NB82-NADA-3018
Sponsored by Department of Energy, Washington, DC. Office of Solar Heat Technologies.

Keywords: *Thermal measurements, Test equipment, Performance tests, Mathematical models, Efficiency, Irradiance, Temperature, Predictions, *Solar water heating, *Solar collectors.

An investigation was carried out to evaluate a possible alternative test method for integral collector storage solar hot water systems. The new test method is an alternative to the established consensus standard method which requires that integral collector storage systems be tested using a solar irradiance simulator. The concept behind the alternative method is to characterize the thermal performance of the solar collection elements in the integral system using standard test methods for conventional solar collectors. After measuring the efficiency and incident angle response, the integral collector storage hot water system would be tested using an electrical heat source to simulate the absorbed solar energy. The research included both experimental and analytical investigations on the col-

lector elements and on the complete system. All-day tests were performed on two commercial integral collector storage solar domestic hot water systems. Tests were performed under a variety of ambient conditions and irradiance levels. An analytical model was developed to predict the thermal performance of one of the systems. Predicted performance was compared with experimental results.

501,120
PB85-187334 Not available NTIS
National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.
Acoustoelastic Evaluation of Arbitrary Plane Residual Stress States in Nonhomogeneous, Anisotropic Plates.
R. B. King, and C. M. Fortunko. Nov 83, 3p
Pub. in Ultrasonics 21, n6 p256-258 Nov 83.

Keywords: *Residual stress, Theories, Normal stress, Velocity measurement, Nondestructive tests, Determination of stress, Evaluation, Homogeneity, Secondary waves, Reprints, *Anisotropic plates, *Ultrasonic tests.

In this paper, it is shown that relative ultrasonic velocity measurements can be used to determine the difference of normal stress components in non-homogeneous, anisotropic plates containing arbitrary residual stress states. Previously the theory relating the velocity of Shear-waves to stress and material anisotropy was limited to the case where the principal directions of stress are parallel to the axes of material symmetry. In this paper, the authors remove this restriction by extending the theory. They also suggest possible experimental procedures for validating the new theory.

501,121
PB85-187417 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Modern Developments in Wind Engineering: Part 3.
Final rept.,
E. Simiu. 1982, 9p
See also PB82-118084.
Pub. in Engineering Structures 4, n2 p66-74 1982.

Keywords: *Wind pressure, *Structural engineering, Stacks(Exhaust), Chimneys, Mathematical models, Dynamic response, Measurement, Aeroelasticity, Fluid flow, Vortices, Reprints.

The paper presents a review of fundamental research on the across-flow response of cylindrical structures immersed in a steaming fluid, and of practical procedures for the estimation of the across-wind response of vertical structures such as chimneys and stacks with circular cross-sections. The results obtained by using the procedures reviewed in the paper are compared with reported measurements of the response of a full-scale tapered chimney. This comparison shows that improvements are needed in the modeling of the across-wind response of chimneys and stacks.

501,122
PB85-196400 PC A02/MF A01
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Building Technology.
Monitoring of Dynamic Response of Floor in 'D' Wing of the Main Building, Bureau of Engraving and Printing.
F. Y. Yokel, and P. W. Mayne. Mar 85, 15p NBSIR-85/3126
Sponsored by Bureau of Engraving and Printing, Washington, DC. Prepared in cooperation with Law Engineering Testing Co., McLean, VA.

Keywords: *Dynamic structural analysis, *Public buildings, Vibration, Floors, Structural engineering, Degradation.

In December 1981, the National Bureau of Standards investigated structural vibrations induced in the first floor of the 'D' wing of the main building of the Bureau of Engraving and Printing. In January 1985, additional measurements were performed to check whether there are any changes in the response characteristics of the floor systems which might indicate structural degradation. The results of these measurements are presented.

501,123
PB85-196541 PC A07/MF A01
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Building Technology.

Research and Innovation in the Building Regulatory Process: Proceedings of the NBS/NCSBCS Joint Conference (6th), Technical Seminar on Streamlined Administrative Procedures, Computers in Construction, and Fire Safety Technology Held at Denver, Colorado on September 11, 1984. Final rept., L. Beavers. Apr 85, 145p NBS/SP-694. See also PB85-196558 through PB85-196640 and PB81-219321. Sponsored by National Conference of States on Building Codes and Standards, Inc., Herndon, VA. Also available from Supt. of Docs as SN003-003-02642-5. Library of Congress catalog card no. 85-600521.

Keywords: *Buildings, *Regulations, *Meetings, Building codes, Structures, Construction, Fires, Safety, Automation, Energy, Design, Warning systems, Compliance, Computer applications.

The Proceedings of the Sixth NBS/NCSBCS Joint Conference on Streamlined Administrative Procedures, Computers in Construction, and Fire Safety Technology contain 10 technical papers: Common Format for the Model Building Codes: An Application of Advanced Techniques for Standards Analysis, Synthesis and Expression; Structural Safety Assessment During the Construction Phase Automation of the Building Code Compliance; Microcomputer Design Tool to Aid Construction Professionals to Comply with the Florida Model Energy Efficiency Code; Automated Checking of Simply-Supported Prismatic Reinforced Concrete Beams for Compliance With Code Requirements; Emerging Engineering Methods Applied to Regulatory Fire Safety Needs; Survey of the State of the Art of Mathematical Fire Modeling; A Second Look at Fire Protection Code Criteria; Non-Evacuation in Compartmented Fire Resistant Buildings Can Save Lives and It Makes Sense; Telephone Connected Early Warning and Communication System.

501,124
PB85-196558

(Order as PB85-196541, PC A07/MF A01) National Bureau of Standards (NEL), Gaithersburg, MD. Center for Building Technology. **Common Format for the Model Building Codes: An Application of Advanced Techniques for Standards Analysis, Synthesis and Expression**, F. I. Stahl. Apr 85, 24p. Sponsored by National Conference of States on Building Codes and Standards, Inc., Herndon, VA. Included in Research and Innovation in the Building Regulatory Process: Proceedings of the NBS/NCSBCS Joint Conference (6th), Technical Seminar on Streamlined Administrative Procedures, Computers in Construction, and Fire Safety Technology held at Denver, Colorado on September 11, 1984, p3-28 Apr 85.

Keywords: *Building codes, *Standards, Classifications, Regulations, Variability, *Format, Data bases, Computer software.

Current research at the NBS Center for Building Technology (CBT) supports development of a common format for the model building codes. This study demonstrates an application of advanced techniques for standards analysis, synthesis and expression (SASE) to code format development. Specifically, the SASE techniques allow model code provisions to be stored in specialized databases, classified for easy access, and displayed in conjunction with any candidate code format. By 'mapping' the technical contents of existing model codes onto various candidate formats, each candidate may be evaluated as to the extent to which it adequately contains and provides access to code provisions. Moreover, the mapping technique permits analysts to determine whether or not the provisions of any individual code have been properly or logically classified. Results of CBT's research will facilitate the more rational development of a common format for model building codes.

501,125
PB85-196566

(Order as PB85-196541, PC A07/MF A01) Arkansas State Univ., State University. **Structural Safety Assessment during the Construction Phase**, T. J. Parsons. Apr 85, 7p. Sponsored by National Bureau of Standards (NEL), Gaithersburg, MD. Center for Building Technology, and National Conference of States on Building Codes and Standards, Inc., Herndon, VA. Included in Research and Innovation in the Building Regulatory Process: Proceedings of the NBS/

NCSBCS Joint Conference (6th), Technical Seminar on Streamlined Administrative Procedures, Computers in Construction, and Fire Safety Technology held at Denver, Colorado on September 11, 1984, p29-35 Apr 85.

Keywords: *Safety, *Structures, *Construction, Loads(Forces), Reinforced concrete, Buildings, Shoring.

A technique is proposed which can be used with reasonable accuracy to determine the effects construction loads have on the structure capacity of a reinforced concrete building. The technique accounts for different types of slab construction, variations in concrete strength throughout the structure, and the nature of different shoring and reshoring systems. The technique uses the equivalent frame method to determine moments and shear forces produced in the structure by the imposed construction loads, and compares these resultants to the shear and moment capacity of the structure at various stages of construction.

501,126
PB85-196590

(Order as PB85-196541, PC A07/MF A01) Atkinson-Noland and Associates, Inc., Boulder, CO. **Automated Checking of Simply-Supported Prismatic Reinforced Concrete Beams for Compliance with Code Requirements**, J. L. Noland, and R. Bedell. Apr 85, 12p. Sponsored by National Bureau of Standards (NEL), Gaithersburg, MD. Center for Building Technology, and National Conference of States on Building Codes and Standards, Inc., Herndon, VA. Included in Research and Innovation in the Building Regulatory Process: Proceedings of the NBS/NCSBCS Joint Conference (6th), Technical Seminar on Streamlined Administrative Procedures, Computers in Construction, and Fire Safety Technology held at Denver, Colorado on September 11, 1984, p71-82 Apr 85.

Keywords: *Beams(Supports), *Reinforced concrete, *Building codes, Automation, Regulations, Design, *Compliance.

Building regulations in their various forms are an important part of the construction industry because they establish standards of quality which are intended to assure at least minimal levels of performance and safety. Automated constraint processing, i.e., checking the characteristics of a given design against the minimum characteristics required by regulation via computer, permits extensive and complex regulations to be more comprehensively and accurately utilized.

501,127
PB85-196608

(Order as PB85-196541, PC A07/MF A01) National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research. **Emerging Engineering Methods Applied to Regulatory Fire Safety Needs**, H. E. Nelson. Apr 85, 9p. Sponsored by National Conference of States on Building Codes and Standards, Inc., Herndon, VA. Included in Research and Innovation in the Building Regulatory Process: Proceedings of the NBS/NCSBCS Joint Conference (6th), Technical Seminar on Streamlined Administrative Procedures, Computers in Construction, and Fire Safety Technology held at Denver, Colorado on September 11, 1984, p83-91 Apr 85.

Keywords: *Fire protection, *Building codes, Design, Buildings, Safety.

The development of fire science has progressed to a point where an analytical engineering methodology for fire protection design is emerging. This presentation outlines the elements of such a method and provides an example of one facet and a broad range of references for those interested in deeper examination.

501,128
PB85-196624

(Order as PB85-196541, PC A07/MF A01) Maryland Dept. of Economic and Community Development, Annapolis. **Second Look at Fire Protection Code Criteria**, D. Hammerman. Apr 85, 4p. Sponsored by National Bureau of Standards (NEL), Gaithersburg, MD. Center for Building Technology, and National Conference of States on Building Codes and Standards, Inc., Herndon, VA.

Included in Research and Innovation in the Building Regulatory Process: Proceedings of the NBS/NCSBCS Joint Conference (6th), Technical Seminar on Streamlined Administrative Procedures, Computers in Construction, and Fire Safety Technology held at Denver, Colorado on September 11, 1984, p113-116 Apr 85.

Keywords: *Fire protection, *Building codes, Fire safety, Design, Buildings, Construction, Regulations.

Building codes and fire codes have placed a great deal of emphasis on fire safety design criteria. Fire safety criteria in the codes are the accumulation of provisions based upon the role of judgment and gathering of historical and scientific data. And this approach has not been without considerable gain in the prevention of fires and reduction in the loss of life in buildings. Recognizing the lack of sophisticated fire data of years ago, it is apparent that the entire subject of building construction classifications and building size limitations must be studied to produce more scientifically-based results.

501,129

PB85-200087 PC A04/MF A01 National Bureau of Standards (NEL), Gaithersburg, MD. Center for Building Technology. **Influence of Block and Mortar Strength on Shear Resistance of Concrete Block Masonry Walls**, K. Woodward, and F. Rankin. Apr 85, 74p NBSIR-85/3143

Keywords: *Masonry, *Concrete blocks, *Walls, Failure, Tests, Mortars(Materials), Shear strength, Axial stress.

Data from seventeen masonry wall panel tests are presented. All of the walls are ungrouted, unreinforced, and constructed with hollow concrete block. The primary variables in the test series are block and mortar strength, but the applied vertical compressive stress and wall aspect ratio are also varied. The walls are built with either a 'high' strength block or a 'low' strength block having gross area unit strengths of approximately 1800 psi and 1300 psi, respectively. The mortar is either a Type S or Type N mortar and, for convenience, is identified as high and low strength mortar, respectively. Thirteen of the wall panels have nominal dimensions of 64 in. long x 64 in. high x 8 in. thick, but two of the walls are 96 in. long and the remaining two walls are 48 in. long. The applied net area vertical compressive stress is constant for a given test, but varies between 100 psi and 400 psi for tests in the series reported herein. The walls are tested in the NBS Tri-directional Test Facility using fixed-ended boundary conditions at the top and bottom of the walls. A vertical compressive stress is applied and maintained while in-plane lateral displacements are imposed at the top of the wall.

501,130

PB85-201770 Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Center for Building Technology. **Computers in Building: A Strategy for Building Research**. Final rept., R. N. Wright. 1984, 7p. Pub. in Building Research and Practice 12, n1 p14-20 Jan-Feb 84.

Keywords: *Buildings, Automation, Research, Computation, Construction, Reprints, *Computer applications, Computer aided design.

Advances in technologies of electronic computation are revolutionizing practices in all phases of building including design, on-site construction, and end use. These advances have potential for increasing the usefulness, safety and economy of buildings. Some current research, development and applications are cited to illustrate the advances in building practices that electronic computation can provide. Expectations are presented for computer-integrated building practices. Research, in traditional and in new areas, required to realize these expectations is described.

501,131

PB85-202729 Not available NTIS National Bureau of Standards (NEL), Gaithersburg, MD. Center for Building Technology.

Field 13—MECHANICAL, INDUSTRIAL, CIVIL, AND MARINE ENGINEERING

Group 13M—Structural Engineering

Computers in Buildings, Building and Building Research.

Final rept.,
R. N. Wright. 1984, 17p
Pub. in Proceedings of Triennial Congress of the Int. Council for Building Research, Studies and Documentation, Stockholm, Sweden, August 1983, p77-93.

Keywords: *Buildings, Automation, Research, Computation, Construction, *Computer applications, Computer aided design.

Advances in technologies of electronic computation are revolutionizing practices in all phases of building including design, on-site construction, and end use. These advances have potential for increasing the usefulness, safety and economy of buildings. Some current research, development and applications are cited to illustrate the advances in building practices that electronic computation can provide. Expectations are presented for computer-integrated building practices. Research, in traditional and in new areas, required to realize these expectations is described.

501,132
PB85-205615 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Sites and Services Projects in Seismic Regions.

Final rept.,
E. Simiu. 1984, 6p
Pub. in Jnl. of Archit. Plan. Res. 1, n3 p175-180 1984.

Keywords: *Structural engineering, Earthquakes, Urban development, Wind pressure, Buildings, Developing countries, Reprints, *Earthquake engineering, Low cost housing.

It is shown in this note that incremental expansion schemes pose special and delicate structural design problems that arise from the evolutionary nature of the building process in sites and services projects. A first type of problems arises if an initial but incomplete shelter core is provided on the site. In that case efficient ways must be found to ensure the structural integrity of the initial construction. A second type of problem is due to the difficulty of tying successive incremental portions of the dwelling both to the initial construction and among themselves in such a manner as to create systems that are structurally sound at all times. Without due attention to such problems the resulting construction can be unnecessarily uneconomical as well as constituting a serious hazard to life and property in case of earthquake or tropical cyclone. The purpose of this note is to illustrate these two types of problems by using examples of shelter construction in actual sites and services projects.

501,133
PB85-205649 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Modern Developments in Wind Engineering. Part 4.

Final rept.,
E. Simiu. 1983, 9p
See also PB85-187417.
Pub. in Engineering Structures 5, n4 p273-281 Oct 83.

Keywords: *Structural engineering, *Wind pressure, Deflection, Buildings, Vibration, Torsion, Reprints.

This is the fourth in a series of review papers devoted to the state-of-the-art in wind engineering. Previous papers were published in the October 1981 and January 1982 issues of Engineering Structures. This paper presents a review of information on along-wind, across-wind, and torsional response of tall buildings, and on the mitigation of wind-induced vibrations through the use of tuned mass dampers.

501,134
PB85-205748 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Measurement of Internal Strain in Cast-Concrete Structures.
Final rept.,
W. C. Stone. 1983, 9p
Pub. in Experimental Mechanics 23, n4 p361-369 Dec 83.

Keywords: *Concrete structures, *Strains, Castings, Finite element analysis, Reprints.

A practical method for experimentally measuring strain profiles inside cast-concrete structures is presented. The technique employs micro-embedment strain gages which are oriented along paths of interest inside the structural element prior to casting. Tests of numer-

ous post-tensioned concrete box girder anchorage elements, and of large-scale pullout test specimens instrumented with micro embedment gages have shown good agreement between the measured strains and those predicted by means of detailed finite element analyses within the linear elastic region of the material.

501,135
PB85-225233 PC A05/MF A01
National Bureau of Standards (NEL), Gaithersburg, MD.

Workshop on Steel Research Needs for Buildings, Held at Gaithersburg, Maryland, March 5-6, 1985.

Final rept.,
C. Culver, N. Iwankiw, and A. Kuentz. May 85, 93p
NBS/SP-693
Library of Congress catalog card no. 85-600546.
Sponsored by National Science Foundation, Washington, DC., American Inst. of Steel Construction, Chicago, IL., and Metal Building Mfrs. Association, Cleveland, OH.

Keywords: *Buildings, *Steel construction, Design, Construction, Fire safety, Loads(Forces), Structural engineering, Earthquake engineering.

This report identifies needed experimental and analytical research to advance the state-of-the-art and improve safety and economy in the design, fabrication and construction of steel buildings. A five year plan for a coordinated research program is included. Recommendations for research projects dealing with the following topics are presented: Total building systems, connections and members, frames, seismic design, load and resistance factor design, fire protection, and design loads. The recommendations were developed at a workshop involving participation by steel industry representatives, design professionals, Federal agency representatives and university researchers.

501,136
PB85-227486 PC A03/MF A01
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Building Technology.

Workshops Convened by the Interagency Committee on Seismic Safety in Construction during 1984.
E. V. Leyendecker, G. E. Turner, and S. G. Fattal.
May 85, 44p NBSIR-85/3161
Also pub. as Interagency Committee on Seismic Safety in Construction rept. no. ICSSC/TR-9. Sponsored by Federal Emergency Management Agency, Washington, DC.

Keywords: *Safety, *Seismic waves, *Construction, *Meetings, Earthquakes, Design, Standards, Building codes, Buildings, Hazards, Earthquake engineering.

In an effort to inform Federal agencies about the most recent development on various earthquake hazards mitigation topics, informal workshops were convened by the Interagency Committee on Seismic Safety in Construction in Washington, DC during 1984. The report presents summaries of the workshop series which included the subjects of implementation of seismic provisions for Federal agencies, lifelines, seismic risk maps, and evaluation of existing buildings. The summaries provide an overview of the major topics discussed. Where applicable, recommendations that resulted are given.

501,137
PB85-227676 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Building Technology.

Data-Base Requirements at the Engineering Stage.
Final rept.,
R. N. Wright. 1985, 6p
Sponsored by National Research Council, Washington, DC. Advisory Board on the Built Environment.
Pub. in Proceedings of Workshop on Advanced Technology for Building Design and Engineering (ABBE), Woods Hole, MA., June 17-22, 1984, p43-48 1985.

Keywords: *Building codes, *Construction, Design standards, Workshops(Meetings), Engineering, Requirements, *Computer aided design.

Data on requirements and engineering standards for design are outlined for discussion and a Workshop conducted by National Research Council Advisory Board on the Built Environment.

501,138
PB85-240448 PC A09/MF A01
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Building Technology.

Building Technology Project Summaries, 1985.
N. Raufaste, and M. Olmert. Jun 85, 177p NBS/SP-446/9
See also PB-261216.

Keywords: *Construction, Bibliographies, Technology, Projects, Abstracts, Buildings, Loads(Forces), Reliability, Thermal analysis, Thermal measurements, Acoustics, Illuminating, Plumbing, Construction materials, Roofing, Concretes, Refrigerants, *Building technology, Earthquake engineering, Solar equipment.

The report summarizes CBT's research for 1985, and is arranged according to CBT's research programs. Each summary lists the project title, its activities, point of contact in CBT, and sponsor. Contents: computer-integrated construction; Structural loads and reliability; Geotechnical engineering; Earthquake engineering; Thermal analysis and measurements; Acoustics; Lighting research; Building controls; Non-Azeotropic refrigerant mixtures research; Test procedures for energy appliances; Solar equipment; Plumbing research; Quality of building materials; Performance of roofing systems; Predicting the performance and service-life of concretes.

501,139
PB86-110111 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Operations Research Div.

Application of the Performance Concept to Fire Safety in Health Care Facilities.

Final rept.,
R. E. Chapman, and W. G. Hall. 1982, 11p
Sponsored by Department of Health and Human Services, Washington, DC.
Pub. in Proceedings of ASTM/CIB/RILEM Symposium (3rd), Lisbon, Portugal, March 29-April 2, 1982, on Performance Concept in Building: Advances in the Development of the Concept and Its Application in Rehabilitation, v1 p481-491.

Keywords: *Fire safety, *Hospitals, Economic analysis, Mathematical programming, Building codes, *Health facilities, Nursing homes.

The identification of cost-effective levels of fire safety in health care facilities is a major concern to hospital administrators, fire safety engineers and public policy makers. The prohibitive costs of strict compliance to the prescriptive provisions of the National Fire Protection Association's Life Safety Code (NFPA 101) in hospitals and nursing homes has led to the development of an equivalency methodology, the Fire Safety Evaluation System. Three topics are described briefly in this paper. They are: (1) The Fire Safety Evaluation System; (2) a mathematical programming procedure which identifies least-cost compliance strategies; and (3) an indication of the cost-saving potential of the Fire Safety Evaluation System.

501,140
PB86-110137 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Structures Div.

Treatment of Accidental Loads and Progressive Failures in Design Standards.

Final rept.,
B. Ellingwood. 1981, 17p
Pub. in Structural Safety and Reliability, p649-665 1981.

Keywords: *Structural design, Loads(Forces), Structural engineering, Building codes, *Structural failure, Structural reliability.

Accidental loads not presently considered in the design of most structures may have catastrophic consequences if they occur. If the structure is not properly designed and detailed, a local failure resulting from the accidental load may initiate a chain reaction of failures throughout a major portion of the structure. The development and implementation of design procedures to control the effects of accidental loads and progressive failures is discussed in the paper. The probability of the initiating event and the probability of a structural failure when the event occurs are both considered. Loading criteria are given for the loads that the damaged structure must carry in order to prevent a progressive failure from initiating from a zone of local damage.

501,141
PB86-110905 PC A05/MF A01
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Building Technology.

Building Technology Publications, Supplement 9: 1984.

Final rept.,
L. Beavers. Aug 85, 76p NBS/SP-457/9
See also PB84-237197.

Keywords: *Construction industry, *Buildings, Abstracts, Structural engineering, Solar heating, Structural design, Construction materials.

The report is the ninth supplement to NBS Special Publication 457, Building Technology Publications, and lists the Center for Building Technology (CBT) documents published during 1984. It includes titles and abstracts of each NBS publication and each paper published in non-NBS media, key word and author indexes, and general information and instructions on how to order CBT publications.

501,142

PB86-111424 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Operations Research Div.

Applications of Equivalency Methodologies to Building Rehabilitation.

Final rept.,
J. H. Pielert, and R. E. Chapman. 1982, 10p
Pub. in Performance Concept in Building: Advances in the Development of the Concept and Its Application in Rehabilitation, v1 p493-502 1982.

Keywords: *Buildings, *Renovating, Building codes, Windows, Doors, Mathematical models, Regulations, Computer aided analysis.

The paper presents the results of a pilot study on the application of an equivalency methodology in achieving regulatory compliance. A computerized procedure is developed which permits the least-cost means of achieving compliance with regulatory provisions applied to windows and doors in buildings being rehabilitated. Application of the methodology to a prototypical townhouse indicated potential savings ranging from 20 to 35 percent.

501,143

PB86-111432 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD.

Removing Regulatory Constraints to Building Rehabilitation.

Final rept.,
J. H. Pielert, and C. J. Dinezio. 1982, 11p
Sponsored by American Society for Testing and Materials, Philadelphia, PA.
Pub. in Proceedings of ASTM/CIB/RILEM Symposium (3rd) on Performance Concept in Building: Advances in the Development of the Concept and Its Application in Rehabilitation, Lisbon, Portugal, March 29-April 2, 1982, v1 p469-479.

Keywords: *Buildings, *Renovating, *Regulations, Building codes, Requirements, Massachusetts.

The paper reports on the formulation of a regulatory concept for the rehabilitation of existing buildings by the National Bureau of Standards in consultation with other representations of the U.S. building community and its implementation by the State of Massachusetts. The proposed regulatory concept discussed in this paper allows rehabilitation of existing buildings without necessarily meeting all new construction code requirements. Recognizing that their statewide building code was a constraint to rehabilitation, Massachusetts developed new code provisions for existing buildings based on this concept. The resulting Article 22 of the State Building Code utilizes a performance approach which allows compliance alternatives in lieu of strict compliance with the prescriptive provisions of the code for new construction. The impact of Article 22 is discussed along with a case study illustration.

501,144

PB86-122843 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Structures and Materials Div.

Predictive Service Life Testing of Structural and Building Components.

Final rept.,
L. W. Masters. 1982, 11p
Pub. in Structural Use of Wood in Adverse Environments, p425-435 1982.

Keywords: *Structural analysis, *Service life, *Structural members, Forecasting, Depreciation, Aging tests(Materials), Buildings, Wooden structures, Evaluation, Reprints, Accelerated life tests.

The paper describes the methodology by which service life data can be obtained and the problems encountered in predicting service life from short-term(or predictive service life) tests. A systematic approach aimed at reducing the problems encountered in predictive testing is described. The approach provides guidelines for evaluating existing predictive service life tests and for developing new, more reliable tests as they are needed. Application of the systematic approach to many components is limited, at present, because of the lack of knowledge regarding exposure conditions and mechanisms of degradation. Despite these limitations, however, the approach is useful in (1) identifying the data needed to develop more definitive tests, (2) ensuring the best possible test is developed, and (3) providing a uniform approach to service life prediction and the reporting of the results.

501,145

PB86-124039 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Structures Div.

Research in Earthquake Hazards Reduction at the National Bureau of Standards.

Final rept.,
E. V. Leyendecker, J. R. Harris, R. N. Wright, and E. O. Pfrang. 1980, 6p
Pub. in Proceedings of World Conference on Earthquake Engineering (7th), Istanbul, Turkey, September 8-13, 1980, v9 p75-80.

Keywords: *Earthquake resistant structures, Seismic design, Building codes, Standards, *Earthquake engineering.

Current and planned Earthquake Hazard Reduction programs for Research and Standards Development at the National Bureau of Standards are being conducted in order to meet the responsibilities assigned to NBS under the President's National Earthquake Hazards Reduction Program. These responsibilities to: (1) provide technical support to the building community in the development of seismic design and construction provisions for building codes and national standards. (2) provide technical support to the Federal agencies in development of seismic design and construction provisions for Federal programs and (3) perform research on performance criteria and supporting measurement technology for earthquake resistant construction, are being carried out in cooperation with the Federal and private sectors.

501,146

PB86-125168 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Structures Div.

Wind Loading and Reliability-Based Design.

Final rept.,
E. Simiu, and J. R. Shaver. 1980, 12p
Pub. in Proceedings of International Conference on Wind Engineering (5th), Ft. Collins, CO., July 8-14, 1979, v2 p1281-1291 1980.

Keywords: *Structural design, Design, Wind pressure, Loads(Forces), *Wind engineering, Wind loads.

The implementation of second-moment formats for the design of wind-sensitive structures requires the clarification of a number of questions which are investigated in the paper. These include the dependence of reliability-based criteria upon type of extreme wind distribution; the influence upon such criteria of sampling and observation errors in the estimation of extreme winds, as well as of errors in the estimation of aerodynamic and structural parameters; the relation between safety indices and nominal probabilities of failure; the dependence of member safety upon wind climate; and the validity of linear approximations to the expression for the load factor.

501,147

PB86-135274 PC A09/MF A01
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Building Technology.

Evaluation of the Thermal Integrity of the Building Envelopes of Eight Federal Office Buildings.

R. A. Grot, A. K. Persily, Y. M. Chang, J. B. Fang, and S. Weber. Sep 85, 199p NBSIR-85/3147
Sponsored by Public Buildings Service, Washington, DC. Office of Design and Construction.

Keywords: *Thermal insulation, *Office buildings, Thermal analysis, Measurement, Tests, Air infiltration, Thermography.

Diagnostic test methods were applied to eight federal office buildings in order to assess the applicability of

these measurement methods for determining the thermal integrity of the building envelope. The eight federal office buildings were located in Anchorage, AK; Ann Arbor, MI; Columbia, SC; Fayetteville, AR; Huron, SD; Norfolk, VA; Pittsfield, MA and Springfield, MA.

501,148

PB86-136967 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Structures Div.

Serviceability Limit States: Wind Induced Vibrations.

Final rept.,
B. Ellingwood, and A. Tallin. 1984, 14p
Pub. in Jnl. of Structural Engineering 110, n10 p2424-2437 Oct 84.

Keywords: *Dynamic structural analysis, *Human factors engineering, Buildings, Design, Random vibration, Loads(Forces), Wind pressure, Stiffness, Reprints.

The article summarizes existing data regarding human tolerance of building motion and describes how a simple checking procedure for this serviceability limit state might be developed using random vibration theory to relate the fluctuating wind forces to structural response.

501,149

PB86-139771 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Operations Research Div.

Cost Impact of the NEHRP (National Earthquake Hazards Reduction Program) Recommended Provisions on the Design and Construction of Buildings.

Final rept.,
S. F. Weber. 1985, 19p
Sponsored by Federal Emergency Management Agency, Washington, DC.
Pub. in Societal Implications: Selected Readings, p1-1 - 1-19 1985.

Keywords: *Building codes, *Construction costs, *Cost analysis, Design standards, Regulations, Safety factor, Earthquake resistant structures, Reprints.

The paper provides some information on the approximate cost impacts resulting from implementation of the NEHRP (National Earthquake Hazards Reduction Program) Recommended Provisions (Building Seismic Safety Council 1984 a) and proposes research to obtain improved estimates of cost impacts. The information is derived from the 52 case studies of the Building Seismic Safety Council (BSSC) trial design program conducted in 1983-84 and based on an amended version of the Applied Technology Council's Tentative Provisions for the Development of Seismic Regulations for Buildings (ATC Tentative Provisions).

501,150

PB86-140332 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD.

Economic Considerations in Insulating Masonry and Wood-Frame Walls of Single-Family Housing.

Final rept.,
S. R. Petersen. 1979, 19p
Sponsored by American Society of Heating, Refrigerating and Air-Conditioning Engineers, Inc., Atlanta, GA., and Department of Energy, Washington, DC.
Pub. in Proceedings of the American Society of Heating, Refrigerating and Air-Conditioning Engineers/Department of Energy-Oak Ridge National Laboratory Conference on Thermal Performance of the Exterior Envelopes of Buildings, Kissimmee, Florida, December 3-5, 1979, p522-540 1981.

Keywords: *Residential buildings, *Economic analysis, Walls, Insulation, Masonry, Evaluation.

Maximum economic levels of insulation in masonry walls are expected to be lower than those for wood-frame walls in many parts of the United States for two distinct reasons: (1) insulation costs are significantly higher for masonry walls, and (2) energy savings are somewhat lower because of differences in the dynamic thermal performance of the two wall types. The report examines the impact of both of these factors in determining economically optimal insulation levels for several types of wall construction used in single-family housing, over a wide range of geographic locations.

Field 13—MECHANICAL, INDUSTRIAL, CIVIL, AND MARINE ENGINEERING

Group 13M—Structural Engineering

501,151

PB86-141926

PC A03/MF A01

National Bureau of Standards (NEL), Gaithersburg, MD. Building Physics Div.

Validation Tests of an Earth Contact Heat Transfer Algorithm,

G. N. Walton. Oct 85, 34p NBSIR-85/3201

Sponsored by Department of Energy, Washington, DC. Office of Solar Heat Technologies.

Keywords: *Buildings, Heat transfer, Algorithm, Experimentation, Tests.

Experimental tests and numerical calculations are performed to determine the suitability of including a simplified earth contact heat transfer algorithm in building energy analysis computer simulations. Reasonable agreement is shown between the finite difference test program and the simplified method. There is very good agreement between the floor surface temperature of the NBS Passive Solar Test Facility and the temperature predicted by the test program.

501,152

PB86-166998

PC A04/MF A01

National Bureau of Standards (NEL), Gaithersburg, MD. Center for Building Technology.

Roof Management Programs,

W. J. Rossiter, W. C. Cullen, and R. G. Mathey. Nov 85, 61p NBSIR-85/3239

Prepared in cooperation with Cullen (William C.) Associates, Potomac, MD. Sponsored by Postal Service, Washington, DC.

Keywords: *Roofs, *Construction management, Roofing, Design, Maintenance.

Roof management programs are used by private and public sector organizations in the United States to help assure that low-sloped roofing systems will perform as intended over their intended service lives. This report reviews those programs. Three general types of roof management programs are identified and discussed. The three types of roof management program currently conducted are: (1) total roof management which treats the design, construction, and maintenance of new and existing roofing; (2) new construction management dealing with design and installation; and (3) maintenance management which considers the maintenance and repair of existing roofs. Four elements are considered essential to an acceptable roof management program: (1) the roof system criterion; (2) quality assurance; (3) quality control; and (4) responsibility. In addition to the roof management programs that have been developed in the private and public sectors, several companies have organized to provide owners with total or partial roof management services.

The common theme that ties together benefit-cost (BC), life-cycle (LCC), and value engineering (VE) analyses is that each is concerned with improving the allocation of resources. This overview of Session A defines some of the common types of economic analysis approaches used in building evaluations, discusses both how they are alike and different, identifies problem areas, and describes current research to overcome those problems. The overview is intended to provide some perspective of how the different types of analyses are related. Papers in Session A are cited to illustrate the points made in the overview.

14B. Laboratories, Test Facilities, and Test Equipment

501,154

PATENT-4 491 014

Not available NTIS

Department of the Army, Washington, DC.

Bond Testing Apparatus.

Patent,

J. F. N. Seiler. Filed 12 Nov 82, patented 1 Jan 85, 5p PB86-174521, PAT-APPL-6-441 310

This Government-owned invention available for U.S. licensing and, possibly, for foreign licensing. Copy of patent available Commissioner of Patents, Washington, DC 20231 \$1.00.

Keywords: *Test equipment, *Patents, *Bonding, Laminates, Substrates, PAT-CL-73-150.

An apparatus for measuring the strength of a bond between a lamina and its substrate, or the like is shown and described. Air, or some other fluid under pressure, causes a gasket to protrude from a piston to seal the atmosphere from a chamber within the piston and the adjacent exposed lamina surface. The fluid also pressurizes this chamber to pull a loading fixture and a portion of the lamina attached thereto away from the substrate. The force required to pull the lamina from the substrate is equal to the strength of the bond.

501,155

PATENT-4 499 770

Not available NTIS

Department of Commerce, Washington, DC.

Systems for Monitoring Changes in Elastic Stiffness in Composite Materials.

Patent,

R. D. Kriz. Filed 22 Jul 82, patented 19 Feb 85, 6p PB85-176550, PAT-APPL-6-400 571

Supersedes PB83-108779.

This Government-owned invention available for U.S. licensing and, possibly, for foreign licensing. Copy of patent available Commissioner of Patents, Washington, DC 20231 \$1.00.

Keywords: *Patents, *Ultrasonic tests, *Fiber composites, Monitoring, Elastic properties, Stiffness, Degradation, PAT-CL-73-599.

Traversing energy flux transmitted into a fiber/matrix composite structure is propagated through the structure in directions which vary depending upon the elastic stiffness condition of the composite. Degradation in elastic stiffness of the composite, from any cause, will result in variations in the direction of travel of the flux through the composite. By determining the direction of flux propagation in the composite, or the portion of the composite structure from which the flux is detected as it exists the structure, the condition of the composite structure, independent of the source of degradation, can be determined. In preferred embodiments the energy flux is ultra-sound energy, while in preferred testing devices a single transmitting transducer is directed towards at least two receiving transducers, for example, one located at a position to receive some flux in the total absence of stiffness degradation, and a second located at a position to receive some flux which would have traveled through a stiffness degraded structure.

501,156

PB85-127421

PC A03/MF A01

National Bureau of Standards, Gaithersburg, MD. Public Information Div.

NBS (National Bureau of Standards) Research Reports.

Special pub.

Oct 84, 32p NBS/SP-680/1

Library of Congress catalog card no. 84-601124.

Keywords: *Research projects, Communications, Automation, Computers, Industries, Mapping, *National Bureau of Standards.

Contents:

Focus on cooperation and communication;
an introduction;
Research updates;
Standard interfaces key to factory automation;
Standard data formats:
transferring part designs between systems;
How to secure your computer systems;
Cold circuits next step in electronics revolution;
New particles for measuring pigments, flour, blood cells;
Measurement methods for a new industry:
industrial radiation;
Compositional mapping:
NBS researchers take a glimpse into the atomic world;
Tools of the NBS compositional mapping program;
New publications;
Conference calendar.

501,157

PB85-172518

Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

Legal Metrology: How the National Bureau of Standards and ASTM Get Involved.

Final rept.,

D. R. Mackay. Dec 84, 7p

Pub. in ASTM (American Society for Testing and Materials) Standardization News 12, n12 p28-30 Dec 84.

Keywords: *Metrology, Law(Jurisprudence), Reprints, *Legal metrology, *International Organization of Legal Metrology, American Society for Testing and Materials, National Bureau of Standards.

This paper describes the International Organization of Legal Metrology (OIML), its objectives and its procedures for the development of International Recommendations. The involvement of the United States in this treaty organization is explained as is the development of U.S. positions on OIML documents. The interface between U.S. OIML activities and ASTM technical committee activities is described for medical instruments, pollution, temperature, and mechanical testing. The potential for future work is described for three areas. A summary of U.S. participation in OIML work is provided and a response is solicited from ASTM members who are interested in the work described.

501,158

PB85-177921

PC A03/MF A01

National Bureau of Standards (NEL), Gaithersburg, MD. Center for Electronics and Electrical Engineering.

Preparation and Certification of SRM's (Standard Reference Materials) for Calibration of Spreading Resistance Probes.

Final rept.,

J. R. Ehrstein. Jan 85, 43p NBS/SP-260/93

Also available from Supt. of Docs as SN003-003-02633-6. Library of Congress catalog card no. 84-601158.

Keywords: *Silicon, *Calibrating, Electrical resistivity, Single crystals, Electrical measurement, *Standard reference materials, *Spreading resistance, *Semiconductors, Chips(Electronics), Uncertainty.

This Special Publication describes the material selection, characterization, data analysis, and measurement process control procedures for four types of Standard Reference Materials (SRMs), available from the National Bureau of Standards, for calibration of spreading resistance measurements on semiconductor silicon. Each of the four comprises a single combination of silicon conductivity-type and crystallographic orientation and contains 16 rectangular silicon chips which are certified for resistivity value based on four-probe resistivity measurements on the slices from which they were cut. The resistivity values of the chips in each set range from about 0.001 ohm-cms to about 100 ohm-cms. The uncertainty of the certified resistivity, as it applies to any individual chip, depends both on the uniformity of the starting slice and on the inherent measurement process uncertainty. The procedure for determining this uncertainty, which is specifically evaluated and tabulated on the certificate for each SRM set, is described.

14. METHODS AND EQUIPMENT

14A. Cost Effectiveness

501,153

PB86-122827

Not available NTIS

National Bureau of Standards (NEL), Gaithersburg, MD. Operations Research Div.

Benefit-Cost Analysis, Life-Cycle Costing and Value Engineering.

Final rept.,

H. E. Marshall. 1984, 9p

Pub. in Proceedings of International Symposium on Building Economics (3rd), Ottawa, Canada, July 18-20, 1984, p15-23.

Keywords: *Benefit cost analysis, Cost analysis, Value engineering, Evaluation, Buildings, Economic analysis.

501,159
PB85-177954 PC A07/MF A01
 Virginia Polytechnic Inst. and State Univ., Blacksburg.
 Dept. of Mechanical Engineering.
Thermal Flanking Loss Calculations for the National Bureau of Standards Calibrated Hot Box,
 R. J. Onega, and P. J. Burns. Feb 85, 149p NBSIR-83/2804
 Sponsored by Department of Energy, Washington, DC.
 Prepared in cooperation with Colorado State Univ., Fort Collins. Dept. of Mechanical Engineering.

Keywords: *Heat loss, *Test chambers, Calibrating, FORTRAN, Heat transmission, Heat measurement, Walls, Computer programs, Mathematical models, Finite difference theory.

A two-dimensional, finite-difference model was developed to calculate the flanking loss for the NBS Calibrated Hot Box. A new definition of flanking loss is presented, along with the thermal theory, a description of the computer code and some results. This model applies to both steady-state and dynamic boundary conditions.

501,160
PB85-178317 PC A05/MF A01
 National Bureau of Standards, Gaithersburg, MD.
 Office of Product Standards Policy.
NVLAP (National Voluntary Laboratory Accreditation Program) Directory of Accredited Laboratories, 1984.
 Rept. for Jan-Dec 84,
 H. W. Berger. Feb 85, 83p NBS/SP-687
 See also PB84-109875. Library of Congress catalog card no. 84-601165.

Keywords: *Directories, *Laboratories, Acceptability, Test facilities, Standards, Tests, *Accreditation, *National Voluntary Laboratory Accreditation Program.

Laboratories accredited by the National Voluntary Laboratory Accreditation Program (NVLAP) are identified along with the specific test methods for which they are accredited. The current status of existing accreditation programs is given for laboratories that test thermal insulation, freshly mixed concrete, carpet, wood burning stoves, paint, and personnel radiation dosimeters, and that provide acoustical testing services. Indexes are provided for searching the Directory for laboratories accredited in specific testing areas or for specific test methods.

501,161
PB85-178432 PC A15/MF A01
 National Bureau of Standards, Gaithersburg, MD.
National Conference on Weights and Measures (69th), 1984,
 A. D. Tholen, L. E. Barbrow, and A. P. Heffernan.
 Jan 85, 342p NBS/SP-684
 See also PB82-178997. Also available from Supt. of Docs as SN003-003-02637-9. Library of Congress catalog card no. 26-27766.

Keywords: *Metrology, *Meetings, Size determination, Metric system, Packaging, Standards, Weight measurement, Tolerances(Mechanics), Specifications, Consumer affairs, Marking, Labels, Regulations, Law(Jurisprudence), *Weights and measures, Legal metrology, Metrication.

The theme of the meeting was 'Transferring Technology for Trade: A Team Effort.' Adoption of a NCWM Constitution and By-laws and a new Scales Code were major actions taken by the membership. The new Scales Code, which will be effective January 1, 1986, represented a significant advancement for device control. Other items addressed included such issues as labeling of gasoline-alcohol blends and national type evaluation. Special meetings included those of the Task Force on Package Control, Metrologists' Workshops, the Associate Membership Committee, the Scale Manufacturers Association, the Industry Committee on Packaging and Labeling, the State regional weights and measures associations, and OIML Pilot Secretariat 20 (Prepackaged Products). Reports by the several standing and annual committees of the Conference comprise the major portion of the publication. Also included are the addresses and technical papers delivered by Conference officials and other authorities from Government and industry.

501,162
PB85-178879 PC A04/MF A01
 National Bureau of Standards, Gaithersburg, MD.

State Weights and Measures Laboratories: Program Description and Directory.
 Final rept.,
 H. V. Oppermann. Jan 85, 75p NBS/SP-686
 Supersedes PB85-137651. Library of Congress catalog card no. 84-601142.

Keywords: *Laboratories, *Calibrating, *Measurement, *Directories, *States(United States), Tolerances(Mechanics), *Weights and measures, State agencies.

The National Bureau of Standards receives repeated requests from industry and Federal agencies (e.g., Department of Defense, Nuclear Regulatory Commission) for information about the capabilities of and services provided by State weights and measures laboratories. This directory is a compilation of such information by State, including a description of the services available and fees charged. The directory will be updated annually in January of each year to coincide with the issuance of annual certification of these laboratories.

501,163
PB85-179117
 (Order as PB85-179083, PC A05/MF A01)
 National Bureau of Standards (NML), Gaithersburg, MD. Center for Chemical Physics.
Automated Coupled-Column Liquid Chromatography System for Measuring Aqueous Solubilities of Hydrophobic Solutes,
 J. W. Owens, H. DeVoe, T. J. Buckley, and S. P. Wasik. 11 Oct 84, 8p
 Prepared in cooperation with Maryland Univ., College Park. Dept. of Chemistry.
 Included in Jnl. of Research of the National Bureau of Standards, v90 n1 p41-48 Jan-Feb 85.

Keywords: *Solubility, *Automation, *Laboratory equipment, Solutes, Temperatures, *Coupled column liquid chromatography, Benzene/ethyl, Computer applications, High performance liquid chromatography.

An automated apparatus is described for measuring the aqueous solubility of a sparingly soluble organic compound at many different temperatures. Water is pumped through a generator column packed with a chromatographic support coated with the organic compound, producing a saturated solution. The solute in a measured volume of this solution is extracted with an extractor column and analyzed by high performance liquid chromatography (HPLC). The temperature of the thermostat bath and the operation of the valves and the HPLC are under the control of a microcomputer. Solubility measurements of ethylbenzene obtained with this apparatus have a standard deviation at any one temperature of about 3% of the mean.

501,164
PB85-182574 PC A03/MF A01
 National Bureau of Standards (NEL), Gaithersburg, MD. Electrosystems Div.
Automatic AC/DC Thermal Voltage Converter and AC Voltage Calibration System.
 Final rept.,
 K. J. Lentner, D. R. Flach, and B. A. Bell. Nov 84, 46p NBSIR-84/2973
 Sponsored by Department of Defense Calibration Coordination Group, Redstone Arsenal, AL.

Keywords: *Calibrating, *Electrical measurement, Electric potential, Automation, Alternating current, Thermal voltage converters.

An automatic ac/dc difference calibration system is described which uses direct measurement of thermoelement emfs. In addition to ac/dc difference testing, the system can be used to measure some important characteristics of thermoelements, as well as to calibrate ac voltage calibrators and precision voltmeters. The system operates over a frequency range from 20 Hz to 100 kHz, covering the voltage range from 0.5 V to 1 kV. For all voltages the total measurement uncertainties expected (including the uncertainty of the specific reference thermal converters used) were 50 parts per million (ppm) at frequencies from 20 Hz to 20 kHz, inclusive, and 100 ppm at higher frequencies up to 100 kHz. The results of initial intercomparisons between the new system and the manual NBS calibration system, using single-range, coaxial-type, thermal voltage converters as transfer standards, are reported. The results show that the agreement between the two systems is better than the uncertainties originally expected, since the intercomparison of ac/dc differences differed by no more than 15 ppm.

501,165
PB85-182780 Not available NTIS
 National Bureau of Standards, Gaithersburg, MD.
Ultrasonic Standard Reference Blocks: What future.
 Final rept.,
 G. V. Blessing, and D. G. Eitzen. 1982, 4p
 Sponsored by American Society for Nondestructive Testing, Columbus, OH.
 Pub. in Proceedings of ASNT National Conference (Spring), Boston, MA., March 22-25, 1982, and (Fall), Pittsburgh, PA., October 4-7, 1982, p9-12 1982.

Keywords: *Ultrasonic tests, *Standards, *Reference blocks.

Flat-bottom-hole ultrasonic reference blocks have been used as reference standards in nondestructive testing for many years. A significant document for their application to aluminum is the ASTM standard recommended practice 'Fabricating and Checking Aluminum Alloy Ultrasonic Standard Reference Blocks.' While much effort has been expended to improve this practice, the block echo amplitude tolerances have in fact gradually increased from the original plus or minus 1 dB criteria in 1958 to their present level of plus 2 and minus 3 dB. This interim report will address the principal system variables which have led to these relaxed requirements, and discuss them quantitatively. Experimental results on a particularly unusual reference block set will be presented as an extremum case of block variability due to material properties.

501,166
PB85-182889 Not available NTIS
 National Bureau of Standards, Gaithersburg, MD.
Analysis of Small Current and Potential Fluctuations in Electrochemical Systems: Significance and Applications.
 Final rept.,
 U. Bertocci. 1982, 16p
 Sponsored by American Inst. of Chemical Engineers, New York.
 Pub. in Proceedings of 1982 Annual Meeting of the American Institute of Chemical Engineers, Los Angeles, CA, November 14-19, 1982.

Keywords: *Electrochemistry, *Noise, Reviews, Sources, Spectral analysis.

The paper is a review of the work on electrochemical noise measurements. They are divided into cases where random noise is the input signal, cases where spontaneous fluctuations of the current or potential occur at or near equilibrium, and cases where macroscopic fluctuations of irreversible nature are the source of the noise. The theoretical background experimental results and their interpretation and applications are presented and discussed.

501,167
PB85-182921 Not available NTIS
 National Bureau of Standards, Gaithersburg, MD.
Role of NBS (National Bureau of Standards) Calibrations in Quality Assurance.
 Final rept.,
 B. C. Belanger. 1983, 6p
 Pub. in Proceedings of Annual Technical Conference of American Society for Quality Control (37th), Boston, MA., May 24-26, 1983, paper in 37th Annual Technical Congress Transactions, p337-342.

Keywords: *Quality assurance, *Calibrating, Quality control, Metrology, National Bureau of Standards, Traceability.

Requirements for 'traceability to national standards can be found in a variety of regulations and standards. Since the agencies requiring traceability do not necessarily define or interpret these requirements uniformly, confusion concerning compliance with such requirements is not uncommon. This paper and a companion paper on Standard Reference Materials discuss the traceability issue from the perspective of the National Bureau of Standards (NBS). Traceability is only one aspect of a total quality assurance program. Statistical quality control techniques developed originally for industrial production processes can be employed to ensure accurate measurements on a continuing basis, using either standard reference materials or calibration services, where they are available from NBS or others.

501,168
PB85-183200 Not available NTIS

Field 14—METHODS AND EQUIPMENT

Group 14B—Laboratories, Test Facilities, and Test Equipment

National Bureau of Standards, Gaithersburg, MD.
Performance of the Ohio State University Rate of Heat Release Apparatus Using Polymethylmethacrylate and Gaseous Fuels.
Final rept.,
V. Babrauskas. 1982, 12p
Pub. in Fire Safety Jnl. 5, n1 p9-20 1982.

Keywords: *Polymethyl methacrylate, *Laboratory equipment, *Fire tests, *Calorimeters, Performance evaluation, Plastics, Burning rate, Heat of combustion, Reprints.

Tests with several gases and with horizontal specimens of polymethylmethacrylate (PMMA) plastic were performed in the Ohio State University (OSU) apparatus using two different techniques: (1) standard compensated thermopile measurement and (2) oxygen consumption. Results indicate that the combustion enthalpy is measured substantially completely with the oxygen consumption technique but that for the materials tested a varying 20 to 30 percent loss is seen with the standard method when the calibration is based on methane. Theoretical analysis and diagnostic irradiance and temperature measurements show this to be attributable to the fact that specimen flames impinge upon and heat up portions of the apparatus.

501,169
PB85-183275 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Electrosystems Div.
Discussion of Paper: Analysis of Calibration Arrangements for AC Field Strength Meters.
Final rept.,
M. Misakian. Feb 85, 1p
Pub. in IEEE (Institute of Electrical and Electronics Engineers) Transactions on Power Apparatus and Systems PAS-104, p496 Feb 85.

Keywords: *Field strength, *Calibrating, Measuring instruments, Alternating current, Electric fields, Transmission lines, Reprints, Field strength meters.

The manuscript is a published discussion of a paper which was presented at the IEEE Power Engineering Society 1984 Summer Meeting. The discussion compares the results of model calculations in the paper with experimental measurements made at NBS.

501,170
PB85-183358 PC A05/MF A01
National Bureau of Standards, Gaithersburg, MD.
State Weights and Measures Laboratories: Program Handbook.
Final rept.,
H. V. Oppermann, and J. K. Taylor. Feb 85, 86p
NBS/HB-143
See also PB85-178879. Library of Congress catalog card no. 85-600502.

Keywords: *Laboratories, *Calibrating, *Measurement, *Handbooks, *States(United States), Tolerances(Mechanics), Tests, *Weights and measures, State agencies, National type evaluation program, Certification, Authorization.

State weights and measures laboratories are custodians of measurement standards at the State level that serve as the basis for assuring equity in the marketplace and as reference standards for calibration services for indigenous industry. As part of its program to encourage a high degree of technical and professional competence in such activities, the National Bureau of Standards (NBS) has developed performance standards and formalized procedures for the following two purposes: 1. certification of competence for the production of reliable metrological measurements (principally mass, volume, and length), and 2. authorization to conduct initial evaluation of weighing and measuring devices/systems before their use in commerce. Part I of this Handbook describes the procedures followed by NBS in certifying State weights and measures laboratories for competence. A certified laboratory must satisfy general and specific requirements for each competence area in which certification is desired. Part II of this Handbook describes the procedures followed in authorizing certified State weights and measures laboratories to conduct evaluation of weighing and measuring devices and systems under the National Type Evaluation Program (NTEP).

501,171
PB85-183382 PC A04/MF A01
National Bureau of Standards, Gaithersburg, MD.
Office of Product Standards Policy.

Standards Committee Activities of the National Bureau of Standards - 1984 Highlights.
Final rept.,
K. G. Newell. Mar 85, 53p NBSIR-85/3129
See also PB84-239755.

Keywords: *Standards, Research management, National Bureau of Standards.

This report summarizes NBS standards committee activities and accomplishments during calendar year 1984. It profiles NBS staff participation on outside standards committees and highlights significant technical and individual contributions made by NBS staff. In 1984, 444 staff members (or 28% of NBS' professional, scientific, and technical staff) participated in 1,138 committees of 89 national and international standards organizations.

501,172
PB85-183523 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Future Directions of Ultrasonic NDE Standards in the U.S.
Final rept.,
G. Birnbaum, and D. G. Eitzen. 1982, 6p
Pub. in Proceedings of the World Conference on Non-Destructive Testing (10th), Moscow, USSR, August 23-27, 1982, p267-272.

Keywords: *Ultrasonic tests, Standards, Calibrating.

The purpose of this report is to examine the current status and future requirements for ultrasonic NDE standards and calibrations. Considerations along this line have been discussed previously (1) but much of the emphasis was on an analysis of the subject; here the authors attempt to emphasize the progress on ultrasonic NDE standards and consider three aspects of the subject. (a) The authors review improvements of accepted standards such as those proposed by ASTM, those traceable to NBS, and those widely used in practice. Improvements in these standards, in the underlying theory and in their relation to practice will have significant impact on future systems. (b) The authors consider proposed methods which are new rather than improvements to those considered in (a). (c) Finally, the authors consider standards and calibration needs for evolving and future ultrasonic NDE methods.

501,173
PB85-183531 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Automation of the NBS (National Bureau of Standards) Laser-Raman Microprobe.
Final rept.,
J. J. Blaha, R. L. Myklebust, and E. S. Etz. 1981, 4p
Sponsored by Microbeam Analysis Society, Bethesda, MD.
Pub. in Proceedings of Annual Conference on Microbeam Analysis Society (16th), Vail, CO., July 13-17, 1981 p61-64.

Keywords: *Raman spectroscopy, *Microprobes, *Laboratory equipment, Fortran, Automatic control equipment, *Laser spectroscopy, Computer applications.

Most functions of the NBS laser Raman microprobe have been placed under computer control. The system controls not only the spectrometer and sample stage but also the data acquisition, the data storage and the data display functions. The automation consists of a DECLAB-11/MNC computer interfaced to a JY HG2 optical spectrometer, a PAR SSR photon counter, a Burleigh dual PZT translator stage (inchworm type), and a Houston 2000 stripchart recorder. A series of FORTRAN routines has been developed to control all of the above for the initialization of all parameters and the subsequent data collection sequence. FORTRAN routines are also available for interactive graphic display of spectra on a DEC VT105 terminal or for plotting the spectra on the stripchart recorder.

501,174
PB85-184513 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
New Portable Ambient Aerosol Sampler.
Final rept.,
D. S. Bright, and R. A. Fletcher. 1983, 9p
Pub. in American Industrial Hygiene Association Jnl. 44, n7 p528-536 1983.

Keywords: *Portable equipment, *Samplers, *Aerosols, Design criteria, Performance evaluation, Particle size, Reprints.

The NBS portable ambient aerosol sampler is designed to collect the respirable and inhalable particle size fractions at 6 l/min for 24 hour sampling periods. Particle size fractionation is accomplished with series filters. The collection efficiency of the inlet is measured by wind tunnel comparisons with isokinetic probes.

501,175
PB85-184596 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Low Cost Interferometer System for Machine Tool Applications.
Final rept.,
A. Dorsey, R. J. Hocken, and M. Horowitz. 1983, 3p
Pub. in Precis. Eng. 5, n1 p29-31 Jan 83.

Keywords: *Interferometers, Machine tools, Polarization, Reprints, Laser applications.

A compact low cost laser interferometer system with sub-micron resolution is described and first performance evaluations reported. The off-set adjust from the four photodiode detector system can also provide a sensitive, simultaneous indication of straightness in 2 axes. The prototype laser interferometer system described here uses a standard He-Ne laser as a source for short distance measurements and should cost less than \$1,000. With a more expensive laser, the same system should be useful over larger distances.

501,176
PB85-184711 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
High Temperature Optical Fiber Thermometer.
Final rept.,
R. R. Dils. 1983, 4p
Pub. in Jnl. of Applied Physics 54, n3 p1198-1201 Mar 83.

Keywords: *Temperature measuring instruments, Fiber optics, Single crystals, Sapphire, Gases, Gas turbines, Bandwidth, Reprints, *Thermometers, Optical fibers, High temperature.

A high temperature optical fiber thermometer made from single crystal sapphire has been developed for use from 600 to approximately 2000C. The device consists of a small blackbody cavity which is sputtered on the end of a thin (0.25 mm to 1.25 mm diameter, 0.05 to 0.30 mm long) sapphire fiber, a connecting low temperature fiber and a conventional optical detector. The radiance from the cavity is used to measure its temperature. The present instrument is calibrated at a single temperature and uses the fundamental radiation laws to interpolate to other temperatures. It is accurate and has a high sensitivity and rapid temporal response. There appear to be a number of applications of the device in both science and industry.

501,177
PB85-184737 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Optical Waveguide Photon Plumbing for the Chemistry Lab: Fiber Optics, Waveguides, and Evanescent Waves as Tools for Chemical Analysis.
Final rept.,
I. Chabay. 1982, 10p
Pub. in Analytical Chemistry 54, n9 p1071-1080 1982.

Keywords: *Laboratories, *Chemical analysis, *Fiber optics, *Waveguides, Spectrochemical analysis, Reviews, Reprints, *Evanescent waves, *Optical waveguides.

The use of waveguide optics to facilitate and enhance spectroscopic chemical analysis is becoming increasingly important. In this paper, the basic concepts and terminology of fiber optics, other forms of waveguide, and evanescent waves are discussed. Recent developments which use waveguides and evanescent waves for chemical analysis are reviewed.

501,178
PB85-186963 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Office of Standard Reference Materials.
New Developments in NBS (National Bureau of Standards) Biological and Clinical Standard Reference Materials.
Final rept.,
R. Alvarez, and G. A. Uriano. 1985, 25p
Pub. in Chapter 2 in Biological References Materials: Availability, Uses, and Need for Validation of Nutrient Measurement, p19-43 1985.

Laboratories, Test Facilities, and Test Equipment—Group 14B

Keywords: *Chemical analysis, *Laboratory equipment, *Clinical chemistry, *Standards, Food analysis, Nutrition, Calibrating, Blood analysis, Trace elements, Iodine, Performance evaluation, Reprints, *Standard reference materials, *Biological processes.

The National Bureau of Standards is responsible under Federal statutes for issuing Standard Reference Materials (SRM's) to help improve and assure the accuracy of laboratory tests. For food science and clinical laboratories, three types of SRM's are available: control materials with certified concentrations of constituents for monitoring the accuracy and precision of methods and experimental data; certified high purity materials for preparing primary standard solutions; and instrument performance SRM's for evaluating the performance of devices and instruments, such as spectrophotometers and thermometers.

501,179
PB85-186971 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Mechanical Production Metrology Div.
Simple and Effective Acoustic Emission Source Location System.
Final rept.,
M. Barsky, and N. N. Hsu. Jan 85, 3p
Sponsored by Electric Power Research Inst., Palo Alto, CA.
Pub. in Materials Evaluation 43, n1 p108-110 Jan 85.

Keywords: *Acoustic detectors, Reprints, Acoustic emissions.

A simple acoustic emission (AE) source location system has been designed, constructed, and demonstrated. It will indicate the approximate location of an AE source inside a square area at a fast rate. The system requires no computer support, is totally self-contained, and can be built with inexpensive, readily available integrated circuits.

501,180
PB85-187433 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Standard Technique for Measuring Window Absorption and Other Efficiency Losses in Semiconductor Energy-Dispersive X-Ray Spectrometry.
Final rept.,
R. E. Stone, F. J. Walter, D. H. Blackburn, P. Pella, and H. W. Kraner. 1981, 6p
Sponsored by Nuclear Science Society (IEEE), New York.
Pub. in X-Ray Spectrometry 10, n2 p91-96 1981.

Keywords: *X ray spectrometers, *Semiconductor devices, *Standards, Efficiency, Reprints, Standard reference materials.

A standard technique for measuring window absorption and other efficiency losses in semiconductor x-ray spectrometers is described. This technique is in the process of being adopted as an IEEE and IEC standard. A NBS Standard Reference Material Glass, SRM-477, has been developed to promote broad availability for the standard and method throughout the user community. Measurements are reported which have been made to establish limits on the geometry of the technique and to determine the effectiveness of the method.

501,181
PB85-187458 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Use of LEDs (Light Emitting Diodes) as YAG Laser Simulators.
Final rept.,
M. Young. 1981, 8p
Sponsored by Aeronautical Systems Div., Wright-Patterson AFB, Ohio.
Pub. in Proceedings of Electro-Optics/Laser '81, Anaheim, CA, November 17-19, 1981, p222-229.

Keywords: *Laser beams, *Simulators, Feasibility, *YAG lasers, *Light emitting diodes.

There is wide interest in using light emitting diodes (LEDs) for calibrating and testing detectors designed to measure weak, diffuse YAG laser beams. Differences of coherence and possible other differences have given rise to the question, is such use of an LED either practically or theoretically justifiable. The purpose of this paper is to examine the problem in some detail and to determine, if possible, the conditions under which suitably filtered LED radiation will adequately simulate a laser beam. The author concludes

that, although there are certain areas that require special care, use of an LED as a laser simulator is entirely feasible.

501,182
PB85-187466 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Description and Verification of the Silicon Photodiode Self-Calibrating Procedure.
Final rept.,
E. Zalewski. 1980, 4p
Pub. in Proceedings of Technical Program Electro-Optical Laser Conf. Expo., Boston, MA, November 19-21, 1980, p208-211.

Keywords: *Photodiodes, *Calibrating, Photodetectors, Radiometry, Silicon, Quantum efficiency, Comparison, Power measurement, Self calibration.

The silicon photodiode self-calibration technique is unlike all other high accuracy absolute radiant power measurements in that it is simple to perform and does not require expensive and elaborate equipment. The steps in the self-calibration procedure for measuring the major quantum efficiency losses are described. Two intercomparisons with electrically calibrated cavity radiometers are presented. These were radiant power measurements in the 1 to 3 mW range at 568 and 633 nm. The agreement in each case was better than 0.1% between these two independent measurement techniques.

501,183
PB85-187482 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
SQUID Applications to Geophysics.
Final rept.,
J. E. Zimmerman, H. Weinstock, and W. C. Overton. 1981, 4p
Sponsored by Office of Naval Research, Arlington, VA.
Pub. in Proceedings of the SQUID Applications to Geophysics Workshop, Los Alamos, New Mexico, June 2-4, 1980, p81-84, 1981.

Keywords: *Magnetometers, Superconductors, Refrigerators, Cryogenics, *SQUID devices, *Cryocoolers.

No alternatives to liquid-helium cryostats for SQUID geomagnetic measurements are presently available, but micro-miniature Joule-Thomson and low-power non-magnetic Stirling cryocoolers are being developed for this and similar purposes. With increasing interest and experimental work on the subject during the past year or two, it is likely that demonstrations of feasibility will occur in the moderately near future, and perhaps even a suitable commercial cryocooler in the next few years.

501,184
PB85-187763 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Quality Assurance of Chemical Measurements.
Final rept.,
J. K. Taylor. 1981, 9p
See also PB85-140671.
Pub. in Analytical Chemistry 53, n14 p1588A-1596A 1981.

Keywords: *Quality assurance, *Chemical analysis, Sampling, Tables(Data), Quality control, Reviews, Standards, Reprints, Standard reference materials.

This paper presents an overview of the practices that are considered to be essential for quality assurance of analytical chemical data. Proper attention must be given to planning the work, sampling, and the selection of the methodology, as well as the actual measurement process. Quality control and the development and use of control charts are discussed. The need for data review and adequate documentation are stressed. The role of SRM's for quality assurance is discussed.

501,185
PB85-189280 Not available NTIS
National Bureau of Standards (NEL), Washington, DC. Electrosystems Div.
Measurement Applications. Part 2.
Final rept.,
R. E. Hebner. 1984, 6p
Sponsored by Department of Energy, Washington, DC. Div. of Electric Energy Systems.
Pub. in IEEE (Institute of Electrical and Electronics Engineers) Tutorial Course 84 EH0225-3-PWR, Fiber Optic Applications in Electrical Power Systems, pF5-F10 1984.

Keywords: *Voltage measuring instruments, *Electric current meters, *Fiber optics, Electric potential, Electric current, Measurement, Electric fields, Magnetic fields, Birefringence, Electrooptics, Faraday effect, Kerr magneto-optical effect, Magnetooptics, Space charge, *Optical fibers.

This paper introduces the physics of photonic systems used to measure voltage and currents and some of the engineering aspects of the systems which must be considered in their application. Sensors based on the Faraday effect, the Pockels effect, and the Kerr effect, as well as those based on mechanical effects are presented. The requirements imposed on the optical fibers by the measurement application are discussed. Selected systems are described to highlight various aspects of the measurement approach.

501,186
PB85-189389 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Mechanical Production Metrology Div.
Optical Techniques for On-Line Measurement of Surface Topography.
Final rept.,
T. V. Vorburger, and E. C. Teague. 1981, 23p
Contract NASA-L-4718B
Pub. in Precision Engineering 3, n2 p61-83 Apr 81.

Keywords: *Surface roughness, *Optical measurement, *Nondestructive tests, Polarimetry, Optical interferometers, Reprints, Ellipsometry, Laser applications, Speckle, State of the art, On line systems.

Optical techniques offer great potential for non-destructive and on-line measurements of surface roughness during manufacturing. The current state of the art is reviewed for a number of optical techniques including specular reflectance, total integrated scatter, diffuseness, angular scattering distributions, speckle, ellipsometry, and interferometry. The paper draws the distinction between the more quantitative but slower profiling techniques and less quantitative parametric techniques, which are faster and hence more useful for high-speed monitoring of surfaces. In their present state of the art these parametric techniques are suitable as comparators rather than as true metrological tools. Speckle techniques hold perhaps the greatest potential as accurate, high-speed metrological tools.

501,187
PB85-189405 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Semiconductor Materials and Processes Div.
Ellipsometry System for High Accuracy Metrology of Thin Films.
Final rept.,
G. A. Candela, and D. Chandler-Horowitz. 1984, 7p
Pub. in SPIE 480--Integrated Circuit Metrology 2, p2-8 1984.

Keywords: *Ellipsometers, *Polarimetry, *Thin films, Metrology, Design, Performance, Calibrating, Dimensional measurement, Thickness, Reprints, Reference standards, Refractive index, Computer applications, Semiconductors, Laser applications.

A computer-controlled spectroscopic ellipsometer of high accuracy has been designed and constructed. A theta-two-theta goniometer unit and optical rail system allows various ellipsometric methods to be used to measure the parameters delta and psi. Three important methods under study for accuracy, precision, and speed of measurement are the conventional null method, the rotating analyzer method, and the principal angle method. All the goniometer angles, including the angle of incidence, can be measured to an accuracy of 0.001 deg. The present light sources are two lasers with fixed wavelengths, 632.8 nm and 441.6 nm, in addition to a monochromator that can be used to scan the wavelength range from 190 to 2600 nm. A unique sample alignment system which uses two quadrant detectors has been developed and a simple but very effective nulling scheme is used. This instrument is primarily used for the metrology of semiconductor materials and for the calibration of reference standards for thin film thickness and refractive index.

501,188
PB85-189447 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Chemical Thermodynamics Div.

Field 14—METHODS AND EQUIPMENT

Group 14B—Laboratories, Test Facilities, and Test Equipment

Oxygen Flow Calorimeter for Kilogram-Size Samples of Municipal Solid Waste. Part 2. Trial Combustions of Kilogram-Size Samples.

Final rept.,
A. E. Ledford, R. V. Ryan, M. L. Reilly, E. S. Domalski, and K. L. Churney. 1982, 7p
Sponsored by Department of Energy, Washington, DC.
Pub. in Resources and Conservation 8, p159-165
1982.

Keywords: *Calorimeters, *Enthalpy, *Combustion, Samples, Reprints, *Refuse derived fuels, *Solid wastes, Municipal wastes.

A new calorimeter is being developed at the National Bureau of Standards to determine the enthalpies of combustion of kilogram-size samples of municipal solid waste (MSW) in flowing oxygen near atmospheric pressure. Experiments were carried out to develop a prototype combustor in which pellets of relatively unprocessed MSW can be rapidly and completely burned with minimal scattering of ash. Pellets of up to 2.2 kg mass with ash contents between 20 and 35% have been successfully burned at a rate of 15 minutes per kilogram initial mass with CO/CO₂ ratios not greater than 0.1%.

501,189

PB85-191401 PC A02/MF A01

National Bureau of Standards (NEL), Gaithersburg, MD. Center for Mfg. Engineering.
Interlaboratory Comparison of Force Calibrations Using ASTM (American Society for Testing and Materials) Method E74-74.
Technical note (Final),
R. W. Peterson, L. Jenkins, and R. A. Mitchell. Apr 85, 25p NBS/TN-1211
Also available from Supt. of Docs as SN003-003-02645-0.

Keywords: *Force, *Calibrating, Detectors, Load cells, Comparison.

A comparison of force calibrations performed by the National Bureau of Standards and 27 other laboratories located in the United States is reported. Force sensors of four different capacities were calibrated in both tension and compression, repeatedly by NBS with deadweight and one time each by the other participating laboratories. The force sensor capacities were 0.5, 5, 20, and 100 klbf (2.2, 22, 89, and 445 kN). Deadweight machines (with and without force multiplication) and force sensor transfer standards (used in a testing machine or a loading frame) were the force standards represented in the study. The force calibration procedure used was Method E74-74 of the American Society for Testing and Materials.

501,190

PB85-195949 Not available NTIS

National Bureau of Standards, Gaithersburg, MD.
Raman Microprobe Spectroscopy.
Final rept.,
G. J. Rosasco. 1980, 60p
Pub. in Advances in Infrared Raman Spectroscopy, p223-282 1980.

Keywords: *Raman spectroscopy, Reviews, Design criteria, Performance evaluation, Chemical analysis, Sampling, Laboratory equipment, Reprints, *Raman microprobe spectroscopy.

Developments in Raman microprobe spectroscopy are reviewed. Instrument design and performance are described, formulae which allow estimates of the limits in spatial resolution and detection are presented. Microanalytical applications in the fields of biology, pathology, mineralogy, geology, environmental analysis, industrial quality control and general chemical and materials characterization are reviewed. Formulae for estimating sample heating by absorption of the excitation laser probe beam are presented. Effective sampling volumes for microprobe collection optics are derived. The optical phonon modes of small particles and a theoretical treatment of inelastic scattering by the vibrational modes of small particles are discussed.

501,191

PB85-200061 PC A05/MF A01

National Bureau of Standards, Gaithersburg, MD.
Office of Weights and Measures.

Index to the Reports of the National Conference on Weights and Measures from the First to the Sixty-Ninth (1905 to 1984).

W. G. Mott. Apr 85, 91p NBS/SP-691
Supersedes COM73-50221. Also available from Supt. of Docs as SN003-003-02649-2. Library of Congress catalog card no. 85-600531.

Keywords: *Weight measurement, *Meetings, Technical reports, Indexes(Documentation), *Weights and measures.

This publication comprises a subject index and a speaker index for the Reports of the National Conference on Weights and Measures from the First (1905) through the Sixty-ninth (1984) and supersedes NBS Special Publication 377.

501,192

PB85-200079 PC A02/MF A01

National Bureau of Standards, Gaithersburg, MD.
Office of Product Standards Policy.

NVLAP (National Voluntary Laboratory Accreditation Program) Assessment and Evaluation Manual,
P. S. Unger. Apr 85, 21p NBSIR-85/3137
See also PB85-178317.

Keywords: *Laboratories, Standards, Tests, Test facilities, Manuals, Evaluation, Assessments, *Accreditation, *National Voluntary Laboratory Accreditation Program.

This manual explains the role of an assessor and evaluator under the National Voluntary Laboratory Accreditation Program (NVLAP). Policies, procedures, and techniques for conducting a NVLAP on-site assessment of a testing laboratory are described. Deficiencies (or departures from the accreditation criteria) and the technical evaluation leading to accreditation recommendations are also discussed.

501,193

PB85-200129 PC A06/MF A01

National Bureau of Standards, Gaithersburg, MD.
Journal of Research of the National Bureau of Standards, Volume 90, Number 2, March-April 1985.

1985, 124p
See also PB85-200137 through PB85-200160 and PB85-179042. Also available from Supt. of Docs as SN703-027-00003-2. Library of Congress catalog card no. 63-37059.

Keywords: *Research projects, Fundamental constants, Standards, Laboratory equipment, Hydrogen, Fugacity, Solutions, Superconductors, Critical field, Spectral emittance, Measurements, Holmium oxides.

Contents:

- New results from previously reported NBS fundamental constant determinations;
- Standards for measurement of the critical fields of superconductors;
- Spectral transmittance characteristics of holmium oxide in perchloric acid solution;
- An apparatus for direct fugacity measurements on mixtures containing hydrogen;
- Programs considered in radiation instruments and laboratory system.

501,194

PB85-200137

(Order as PB85-200129, PC A06/MF A01)

National Bureau of Standards, Gaithersburg, MD.

New Results from Previously Reported NBS (National Bureau of Standards) Fundamental Constant Determinations,

B. N. Taylor. 13 Dec 84, 4p
Included in Jnl. of Research of the National Bureau of Standards, v90 n2 p91-94 Mar-Apr 85.

Keywords: *Fundamental constants, *Standards, Faraday effect, Josephson junctions, Hall effect, Measurement, Avogadro constant.

A new treatment of previously reported results of three electric-unit-dependent fundamental constant experiments carried out at NBS over the last decade or so yields accurate, indirect values in SI units for a number of important quantities. These include the fine-structure constant alpha, the Avogadro constant (N_{sup} A), the Josephson frequency-voltage ratio 2e/h, and the quantized Hall resistance R(sup H) = h/sq e.

501,195

PB85-200145

(Order as PB85-200129, PC A06/MF A01)
National Bureau of Standards, Boulder, CO.

Standards for Measurement of the Critical Fields of Superconductors,

F. R. Fickett. 21 Nov 84, 19p
Included in Jnl. of Research of the National Bureau of Standards, v90 n2 p95-113 Mar-Apr 85.

Keywords: *Superconductors, *Critical field, *Standards, Measurement.

The origins, definitions, and measurement of the various critical magnetic fields associated with superconductors are reviewed. The potential need for a consensus standard for the measurement of these fields is evaluated. Measurement techniques as practiced both in industry and in the national laboratories and extrapolation techniques commonly used to determine the upper critical fields of the newer materials are presented. Sources of error in the experimental determination of critical fields are assessed for the various common techniques. A comprehensive bibliography of the modern literature on critical field measurement and interpretation is included.

501,196

PB85-200152

(Order as PB85-200129, PC A06/MF A01)

National Bureau of Standards, Gaithersburg, MD.

Spectral Transmittance Characteristics of Holmium Oxide in Perchloric Acid Solution,

V. R. Weidner, R. Mavrodineanu, K. D. Mielenz, R. A. Velapoldi, and K. L. Eckerle. 28 Nov 84, 11p
Included in Jnl. of Research of the National Bureau of Standards, v90 n2 p115-125 Mar-Apr 85.

Keywords: *Spectral emittance, *Solutions, *Spectrophotometers, Measurement, Visible spectrum, Design criteria, Performance evaluation, Wavelengths, *Holmium oxides.

The work describes the methods and procedures used to determine the wavelengths of minimum transmittance of holmium oxide in perchloric acid solution. Measurements of spectral transmittance of the solutions were made by means of a high precision spectrophotometer over the wavelength range 200 nm to 680 nm. The wavelength scale accuracy of this instrument was verified by extensive measurements of mercury and deuterium emission lines. The measurements of spectral transmittance of the holmium oxide solutions were made as a function of temperature, purity, concentration, and spectral bandwidth. Analysis of the uncertainties associated with these parameters and the uncertainties associated with the calibration of the instrument wavelength scale and the data analysis have resulted in an estimated uncertainty of + or - 0.1 nm for the determination of the wavelengths of minimum transmittance of the holmium oxide solution.

501,197

PB85-200160

(Order as PB85-200129, PC A06/MF A01)

National Bureau of Standards, Boulder, CO.

Apparatus for Direct Fugacity Measurements on Mixtures Containing Hydrogen,

T. J. Bruno. 7 Jan 85, 12p
Included in Jnl. of Research of the National Bureau of Standards, v90 n2 p127-139 Mar-Apr 85.

Keywords: *Fugacity, *Measuring instruments, *Hydrogen, Mixtures, Membranes, Methane, Propane, Partial pressure, Temperature, Gas chromatography, Measurement.

An apparatus has been designed and constructed to allow measurements of fugacities in gaseous mixtures containing hydrogen. The apparatus makes use of a semipermeable membrane to allow a direct measurement of the partial pressure of a permeating component (in this case, hydrogen) in a mixture with a non-permeating component. In this study, measurements were made on mixtures of hydrogen/methane and hydrogen/propane. Using measured values of the mixture pressure, hydrogen partial pressure and mixture mole fraction at a given temperature, fugacity coefficients were determined using the virial equation. The measured values are compared with some previous data and general trends are discussed.

501,198

PB85-200178

(Order as PB85-200129, PC A06/MF A01)

National Bureau of Standards (NML), Gaithersburg, MD. Electricity Div.

Investigation of the Uncertainties of the NBS (National Bureau of Standards) Thermal Voltage and Current Converters.

Final rept.,
F. L. Hermach. Apr 85, 124p NBSIR-84/2903

Keywords: *Standards, *Electrical measurement, Accuracy, Calibrating, Thermoelectric generators, Converters, Transfer standards.

The uncertainties of the NBS reference and working standards for ac-dc current and voltage transfer measurements have been redetermined, to 50 and 100 kHz, respectively, by means of a set of multijunction thermal converters (MJTCs), an improved emf comparator, and extensive series of intercomparisons. Numerous supporting investigations have also been performed. As a result of this work the accuracy of the NBS standards and the output of its calibration service for ac-dc current and voltage transfer are considered to be on a much firmer and better documented basis than heretofore. Improvement by factors of two to five in the calibration accuracy for high-quality, single-range thermoelements and thermal voltage converters is possible for certain ranges of current, voltage, and frequency. For very special tests, such as international comparisons, accuracies approaching 1 ppm are within reach.

501,199

PB85-201507 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.

Heterochromatic Stray Light in UV Absorption Spectrometry: A New Test Method.

Final rept.,
K. D. Mielenz, V. R. Weidner, and R. W. Burke. 1982, 3p
Pub. in *Applied Optics* 21, n18 p3354-3356, 15 Sep 82.

Keywords: *Spectrophotometers, *Ultraviolet spectrophotometers, Estimating, Reprints, Stray light, Test methods.

A new method of estimating the amount of heterochromatic stray light in UV spectrophotometers is described. The method uses the same solution filters with sharp UV absorption edges as ASTM Test Method E387, but one measures the apparent absorbance of a 10-mm pathlength cell in the sample beam relative to a 5-mm cell in the reference beam. Scanning towards shorter wavelengths, one records an apparent absorbance maximum which is a direct measure of the stray light. This method was found to be in satisfactory agreement with the ASTM method in comparative tests of several spectrophotometers at different wavelengths between 200 and 390 nm, using KCl, KI, NaI, acetone, and NaNO₂ solution filters. The new method proved to be simpler, the main advantage being that the apparent absorbance maximum occurs at considerably lower scale values than the corresponding absorbance plateau measured by the ASTM method. This reduces the need for successive attenuations of the reference beam every time the spectrophotometer runs off scale. In many instances the new method required no attenuation at all.

501,200

PB85-201812 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Inorganic Materials Div.

Effect of Multiregion Crack Growth on Proof Testing.

Final rept.,
S. M. Wiederhorn, S. W. Freiman, E. R. Fuller, and H. Richter. 1984, 22p
Sponsored by Office of Naval Research, Arlington, VA. Pub. in *American Society for Testing and Materials, Special Technical Publication* 844, p95-116 1984.

Keywords: *Tests, Crack propagation, Cracks, Glass, Strength, Weibull density functions, Reprints, Fracture(Mechanics).

The effect of subcritical crack growth on proof testing is examined. Crack velocity curves obtained by fracture mechanics techniques are used to predict theoretical strength distributions for specimens that survive proof testing. These theoretical distributions are compared with experimental distributions obtained on soda lime silica glass slides. The comparison reveals a surprising sensitivity of the proof test results to the exact position and shape of the crack growth curve. Minor changes in the crack growth curve results in major shifts in position and shape of the strength distribution curves after proof testing. The importance of crack geometry and specimen configuration to crack growth

behavior, and hence, to the strength distribution is emphasized.

501,201

PB85-201838 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Temperature and Pressure Div.

Pressure and Temperature Measurements in the Annulus Between the Piston and Cylinder of a Simple Dead-Weight Piston Gauge.

Final rept.,
B. E. Welch, and V. E. Bean. Dec 84, 9p
Pub. in *Review of Scientific Instruments* 55, n12 p1901-1909 Dec 84.

Keywords: *Pressure measurement, *Temperature measurement, *Measuring instruments, Pistons, Cylinders, Metrology, Fluid flow, Pressure gradients, Temperature gradients, Accuracy, Reprints.

Precise and fundamental pressure measurements are obtained using piston gages. Elastic distortion of the piston and cylinder is the leading cause of inaccuracy in measurement of higher pressures. The equation used for calculating the distortion contains the ratio of the pressure in the annulus between the piston and the cylinder to the pressure under the piston. As the proper value of this ratio or a method to determine it were unknown, the practice has been to assume a value of 0.5. In this work, the pressure and temperature of the fluid in the annulus has been measured along the working length of the piston and the cylinder. The model for the pressure ratio proposed by Bass on the basis of dimensional metrology is an excellent agreement with the pressure measurements.

501,202

PB85-201846 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Molecular Spectroscopy Div.

High Resolution Raman Spectroscopy of Gases with a Fourier Transform Spectrometer.

Final rept.,
A. Weber, D. E. Jennings, and J. W. Brault. 1984, 4p
Pub. in *Proceedings of Int. Conf. on Raman Spectroscopy* (9th), Tokyo, Japan, August 27-September 1, 1984, p58-61.

Keywords: *Raman spectroscopy, Raman spectra spectra, Spectrometers, Fourier transformation, Performance evaluation, Spectrochemical analysis, *Fourier transform spectroscopy.

An experimental study was undertaken showing for the first time that, contrary to earlier predictions, good quality high resolution Raman spectra of gases can be obtained with a Fourier transform spectrometer. Several improvements in the technique are suggested to further enhance the advantages of Fourier transform Raman spectroscopy over that done with grating spectrographs.

501,203

PB85-201895 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.

Role of Fast Secondary Electrons in Degrading Spatial Resolution in the Analytical Electron Microscope.

Final rept.,
D. C. Joy, D. E. Newbury, and R. L. Myklebust. 1982, 2p
Pub. in *Jnl. of Microscopy* 128, pt. 2, pRP1-RP2 Nov 82.

Keywords: *Chemical analysis, *X ray analysis, *Electron microscopes, Monte Carlo methods, Reprints.

Fast secondary electrons generated by high energy beam electrons scatter at angles which carry them laterally through a thin foil. Monte Carlo electron trajectory simulation of this effect reveals that fast secondary electrons degrade the spatial resolution of analysis by means of analytical electron microscopy. The magnitude of the effect increases as the edge energy of the x-ray of interest decreases.

501,204

PB85-201994 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.

New Spectrograph with a Multichannel Optical Detector for the Raman Characterization of Microparticles.

Final rept.,
F. J. Purcell, and E. S. Etz. 1982, 6p
Sponsored by Microbeam Analysis Society, Bethesda, MD.

Pub. in *Proceedings of Annual Conference of the Microbeam Analysis Society* (17th), Washington, DC., August 9-13, 1982, p301-306.

Keywords: *Raman spectroscopy, *Optical equipment, *Spectrographs, Laboratory equipment, Particles, Performance evaluation, Design criteria, *Laser spectroscopy, Air pollution detection, State of the art.

A new triple spectrograph, developed by a U.S. optical instrumentation firm, has been evaluated in a prototype instrument configuration for low light level Raman scattering experiments from single microparticles. In conjunction with an argon ion laser as a Raman excitation source, an advanced fore-optical microsampling system designed around a microscope, and a state-of-the-art optical multichannel analyzer utilizing a linear diode array detector, the system represents a new type of Raman microprobe. The basic configuration of the system is described with emphasis on the new spectroscopic advances embodied in the prototype instrument. The important performance characteristics are compared to currently used micro-Raman instrumentation employing monochannel, scanning systems. The spectral multiple advantage in the acquisition of micro-Raman spectra is demonstrated with examples from the measurement of laser radiation sensitive microparticles. Highlighted are the advantages of fast data acquisition under conditions of broad spectral coverage. Preliminary results are presented from the analysis of 'real-world' microsamples (e.g., power plant stack particulates). These are placed in the perspective of the current state of the field of micro-Raman spectroscopy.

501,205

PB85-202091 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.

Upholstered Furniture Heat Release Rates: Measurements and Estimating.

Final rept.,
V. Babrauskas. 1983, 24p
Pub. in *Jnl. of Fire Sci.* 1, n1 p9-32 Jan-Feb 83.

Keywords: *Flammability testing, *Calorimeters, *Burning rate, *Upholstery, Textiles, Design criteria, Comparison, Oxygen consumption, Cotton fabrics, Polyurethane, Foam, Reprints.

A new instrument, termed a furniture calorimeter, has been constructed and placed into operation for measuring furniture heat release rates based on oxygen consumption. Using the furniture calorimeter, burning rate information has been obtained on a series of 13 chairs, loveseats, and sofas, most of them specially built to permit direct comparisons of construction features. A quantitative assessment is made of the effect of fabric types, filling types (cotton batting, ordinary polyurethane foam, and California-requirements foam), and frame types. The advantages of furniture calorimeter testing over normal room fire testing are discussed. Based on these measurements, an estimating rule is presented for determining the heat release rate. Finally, implications for achieving both good flaming ignition behavior and good cigarette ignition resistance are discussed.

501,206

PB85-202109 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.

Automated NBS (National Bureau of Standards) 1-Omega Measurement System.

Final rept.,
K. R. Baker, and R. F. Dziuba. 1983, 5p
Pub. in *IEEE (Institute of Electrical and Electronics Engineers) Transactions on Instrumentation and Measurement* 32, n1 p154-158 1983.

Keywords: *Electric measuring instruments, Calibrating, Resistors, Microcomputers, Comparators, Reprints, Computer applications.

A microcomputer controlled measurement system has been developed for calibrating stable, 1-ohm standard resistors. It consists of a direct current comparator potentiometer, a self-balancing detector circuit, and special switching networks. The measurement system is capable of comparing resistors to a precision of better than 0.01 ppm.

501,207

PB85-202596 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.

Field 14—METHODS AND EQUIPMENT

Group 14B—Laboratories, Test Facilities, and Test Equipment

Development of a Personal Exposure Monitor for Two Sizes of Inhalable Particulates.

Final rept.,
R. L. McKenzie, D. S. Bright, R. A. Fletcher, and J. A. Hodgeson. 1982, 5p
Pub. in *Environment International* 8, n1-6 p229-233 1982.

Keywords: *Monitors, *Particles, *Public health, *Air pollution, Exposure, Sampling, Nitrogen dioxide, Concentration(Composition), Wind tunnels, Reprints, *Indoor air pollution, *Air pollution sampling.

Measurement of personal exposure to ambient level particulate concentrations is often extremely difficult because of a lack of personal exposure monitors capable of collecting measurable quantities within a meaningful sampling period. A new personal exposure monitor for two fractions of inhalable particulates (i.e., the 3-15 micrometers aerodynamic diameter and the <3 micrometers or respirable fraction) has been developed and characterized. This monitor is capable of collecting a sample of each fraction that is quantifiable with ambient concentrations of inhalable/respirable particulates as low as 25 micrograms/cu m in a 24-h sampling period. Wind tunnel tests have been made on the particulate personal exposure monitor to determine sampling efficiency as a function of relative wind speed and orientation with respect to the sampler.

501,208 PB85-202661 Not available NTIS

National Bureau of Standards, Gaithersburg, MD.
Optimum Applied Field for Magnetic Particle Inspection Using Direct Current.
Final rept.,
C. L. Oehl, and L. J. Swartzendruber. 1982, 12p
Pub. in *Jnl. of Nondestructive Evaluation* 3, n3 p125-136 Sep 82.

Keywords: *Nondestructive tests, *Magnetic particle tests, Leakage flux, Inspection, Reprints.

Experimental measurements of leakage fields from cylindrical defects were obtained in a geometry which permitted simultaneous measurement of the magnetic induction of the material. The results obtained are compared with calculations using a nonlinear finite difference method. Both the experiments and the calculations indicate that the magnitude of the leakage field continues to grow nearly in proportion with the applied field well into the saturation region of the magnetic material. The implications for magnetic particle inspection are discussed.

501,209 PB85-202851 Not available NTIS

National Bureau of Standards, Gaithersburg, MD.
Performance Characteristics of a Continuum-Source Echelle Wavelength Modulated Atomic Absorption Spectrometer.
Final rept.,
J. D. Messman, M. S. Epstein, T. C. Rains, and T. C. O'Haver. 1983, 4p
Pub. in *Analytical Chemistry* 55, n7 p1055-1058 1983.

Keywords: *Chemical analysis, Standards, Laboratory equipment, Design criteria, Performance evaluation, Continuum mechanics, Spectral lines, Reprints, *Atomic absorption spectrometers, Standard reference materials.

The operational features of a single-channel atomic absorption spectrometer based on a continuum source and an echelle monochromator modified for wavelength modulation (CEWM-AA) are described. Characteristic concentrations, detection limits, and upper concentration limits of approximately 100 spectral lines for 32 elements were experimentally determined by CEWM-AA using air-acetylene and nitrous oxide-acetylene flames. Detection limits of CEWM-AA are generally within an order of magnitude of line-source atomic absorption (AAL) detection limits for those elements with analysis lines above 240 nm. When using optimal lines for CEWM-AA, only Zn, Te, Sb, Cd, and Pd of the 32 elements investigated have detection limits which are inferior to AAL detection limits by more than an order of magnitude. Analyses of several NBS Standard Reference Materials (SRMs) using either flame or graphite electrothermal atomizers demonstrated comparable analytical performance between CEWM-AA and the AAL system operated in the background correction mode (AAL-BC).

501,210 PB85-203446 Not available NTIS

National Bureau of Standards, Gaithersburg, MD. Foreign National Organizations Which Accredited Laboratories that Provide Calibration Services.

Final rept.,
J. W. Locke. 1983, 5p
Sponsored by National Conference of Standards Labs., Silver Spring, MD. Information and Directory Committee.
Pub. in a *Directory of Standards Laboratories* p78-82 1983.

Keywords: *Laboratories, *Calibrating, Reprints, *Foreign technology, Accreditation.

The article lists 13 foreign national laboratory accreditation systems which accredit laboratories that provide calibration services in their country.

501,211 PB85-203453 Not available NTIS

National Bureau of Standards, Gaithersburg, MD.
Measures and Measurement Systems.
Final rept.,
A. O. McCoubrey. 1984, 14p
Sponsored by Grolier, Inc., Danbury, CT.
Pub. in *Encyclopedia Americana*, p584-597 1984.

Keywords: *Units of measurement, *Metric system, *Measurement, Reviews.

The article reviews the history of measurements and the evolution of measurement systems. The development of the metric system is traced from the beginnings to the present International System of Units. The history of measurements in the United States is discussed with attention to the consideration of the metric system and its utilization. The relationship of English and the United States measurement units is described and tables give customary units. The International System of Units is also described and extensive tables are included.

501,212 PB85-203545 Not available NTIS

National Bureau of Standards (NEL), Gaithersburg, MD. Semiconductor Materials and Processes Div.
Effects of Instrumental Artifacts on the Quantitative Determination of Oxygen in Silicon by FTIR (Fourier Transform Infrared).
Final rept.,
A. Baghdadi. 1984, 15p
Pub. in *American Society for Testing and Materials, Special Technical Publication* 850, p343-357 1984.

Keywords: *Chemical analysis, *Oxygen, *Infrared spectroscopy, Silicon, Reprints, *Fourier transform spectroscopy.

The evolution of silicon processing technologies towards greater reliance on internal gettering by oxygen precipitates has led to the need for greater precision in the measurement of the interstitial oxygen content of silicon slices. This measurement is presently being carried out with the use of Fourier Transform Infrared (FTIR) spectrophotometers. This paper concerns the investigation of the effects of changing the apodization function and beam geometry on the quantitative determination of oxygen in silicon by FTIR. The apodization functions used include the boxcar, cosine, Happ-Genzel, and triangular functions. The beam geometry is varied by placing apertures between the interferometer and the silicon specimen. The effects of beam polarization and detector nonlinearity were also investigated.

501,213 PB85-203552 Not available NTIS

National Bureau of Standards (NML), Boulder, CO. Time and Frequency Div.
Coordinate Time on and Near the Earth.
Final rept.,
N. Ashby, and D. W. Allan. 5 Nov 84, 1p
Pub. in *Physical Review Letters* 53, n19 1858p, 5 Nov 84.

Keywords: *Atomic clocks, *Time measurement, General relativity, Synchronism, Reprints, Frequency synchronization, Sagnac effect.

Gravitational frequency shifts, second-order Doppler shifts, and the Sagnac effect are well determined path-dependent relativistic effects which must be considered when synchronizing atomic clocks. Using the coordinate time of General Relativity in a local inertial frame as a basis, and applying appropriate corrections to the readings of atomic clocks and to time delays of

electromagnetic signals, a network of consistently synchronized clocks can be established near the Earth.

501,214 PB85-203560 Not available NTIS

National Bureau of Standards (NML), Gaithersburg, MD. Office of Standard Reference Materials.
Standard Solutions and Certified Reference Materials.
Final rept.,
R. Alvarez. 1984, 8p
Pub. in *Official Methods of Analysis of the Association of Official Analytical Chemists*, Chapter 50, p1002-1009 1984.

Keywords: *Standards, Solutions, Reprints, *Certified reference materials.

No abstract available.

501,215 PB85-205227 Not available NTIS

National Bureau of Standards (NEL), Gaithersburg, MD. Mechanical Production Metrology Div.
Development of High Fidelity Acoustic Emission Transducers.
Final rept.,
T. Proctor, F. Breckenridge, and D. Eitzen. Dec 83, 9p
Sponsored by American Society for Metals, Metals Park, OH.
Pub. in *Proceedings of Int. Conf. NDE in the Nuclear Industry* (6th), Zurich, Switzerland, November 28-December 2, 1983, p329-337.

Keywords: *Transducers, Nondestructive tests, Displacement, Acoustic emission testing.

The development of a transducer which measures the normal displacement of a 'point' on a surface is reviewed. This transducer has sufficient bandwidth so that it can measure, with high sensitivity, the dynamic surface motion due to an AE event. Certain improvements in the design are discussed. Captured waveforms from the best model of the transducer are compared with theoretical elasticity predictions of surface displacement. The transducer will be made available for purchase as a transfer standard through the Standard Reference Materials Program of the National Bureau of Standards. Preliminary results from a new transducer for measuring tangential surface motion are also presented.

501,216 PB85-205243 Not available NTIS

National Bureau of Standards (NEL), Washington, DC. Statistical Engineering Div.
Some Basic Statistical Methods for Chromatographic Data.
Final rept.,
K. Kafadar, and K. R. Eberhardt. 1984, 34p
Pub. in *Advances in Chromatography* 24, p1-34 1984.

Keywords: *Chromatographic analysis, *Statistical analysis, Reviews, Gas chromatography, Mathematical models, Reprints, Liquid chromatography, Reference materials, High performance liquid chromatography.

The article reviews some basic notions of statistics that are applicable particularly for measurements obtained by gas and liquid chromatography. Included in this review are probability models for measurement error, classical and robust methods for obtaining confidence intervals, and the use of analysis of variance and median polish to analyze linear additive models. GC and HPLC data are used to illustrate these techniques, as well as to introduce methods for estimating a drift rate, testing homogeneity of a reference material, and obtaining a valid uncertainty statement from a set of correlated measurements.

501,217 PB85-205334 Not available NTIS

National Bureau of Standards, Gaithersburg, MD. Polymer Science and Standards Div.
Role of Interlaboratory Test Programs in Quality Assurance.
Final rept.,
J. D. Barnes. 1985, 18p
Pub. in *American Society for Testing and Materials Special Technical Publication* 846, p31-48 1985.

Keywords: *Quality assurance, *Plastics, *Tests, Standards, Production methods, Reprints.

A program for assuring the quality of products made from plastics is only as valid as the test methodology that supports it. Test methods can be characterized as to their repeatability and reproducibility. Both of these measures describe the level of precision, or agreement among test results, obtained when a test method is used to characterize a product, be it raw material or a finished part. ASTM requires that each test method in the ASTM Book of Standards be provided with a statement of precision and accuracy. This paper describes some recent efforts within Committee D20 on Plastics to assess the precision of two test methods. The results are analyzed using ASTM Practice for Conducting an Interlaboratory Test Program to Determine the Precision of a Test Methods (E691). The implications of the measured precision of the test methods for their use in quality assurance activities are described.

501,218
PB85-205763 Not available NTIS
 National Bureau of Standards, Gaithersburg, MD.
Practical Limits of Precision in Inductively Coupled Plasma Spectrometry.
 Final rept.,
 R. L. Watters. 1983, 10p
 Pub. in American Laboratory 15, n3 p16-25 1983.

Keywords: *Chemical analysis, *Calibrating, Performance evaluation, Emission spectroscopy, Reprints, *Inductively coupled plasma spectroscopy.

Quantitative analysis using the Inductively Coupled Plasma (ICP) technique involves a series of measurement procedures. In order to evaluate the overall precision of the technique, non-random errors must be eliminated and the random error of each step in the measurement process must be considered. Calibration functions, spectral overlap corrections, blank corrections, and other factors are often treated as nonvariable quantities. Approaches to including the error associated with these steps are presented. Using these approaches will enable the analyst to construct realistic confidence limits on the final ICP results.

501,219
PB85-205805 Not available NTIS
 National Bureau of Standards, Gaithersburg, MD.
Sinusoidal Profile Precision Roughness Specimens.
 Final rept.,
 E. C. Teague, F. E. Scire, and T. V. Vorburger. 1982, 13p
 Pub. in Int. Conf. on Metrology and Properties of Engineering Surfaces (2nd), Leicester, England, April 14-16, 1982, Wear 83, n1-2 p61-73 Dec 82.

Keywords: *Surface roughness, *Roughness, *Calibrating, Metrology, Precision.

The design, specifications, fabrication, testing, and potential use of a series of sinusoidal profile precision roughness specimens are described. These specimens have been designed primarily to provide a means for optimum transfer of an accurate roughness average, ($R_{sub a}$), value from primary to secondary laboratories. However, properties of the specimens also make them very useful for evaluating instrumentation and computational algorithms designed to measure the statistical parameters and functions now being investigated in many laboratories. Specimens with an ($R_{sub a}$) value of 1.0 micrometer and spatial wavelengths of 40, 100 and 800 micrometers are being fabricated. For the 100 micrometer wavelength, specimens are also being fabricated with ($R_{sub a}$) values of 3.0 and 0.3 micrometers. Fabrication with numerically controlled diamond lathes has produced specimens with very high quality sinusoidal profile waveforms, with uniform ($R_{sub a}$) values across the surfaces and with very low amounts of waviness over a test area of about 2 sq cm.

501,220
PB85-205813 Not available NTIS
 National Bureau of Standards, Gaithersburg, MD.
Three Dimensional Stylus Profilometry.
 Final rept.,
 E. C. Teague, F. E. Scire, S. M. Baker, and S. W. Jensen. 1982, 12p
 Pub. in Proceedings of Int. Conf. on Metrology and Properties of Engineering Surfaces (2nd), Leicester, England, April 14-16, 1982, Wear 83, n1-2 p1-12 Dec 82.

Keywords: *Surface roughness, Metrology, *Profilometry, Three dimensional.

Work at the NBS to acquire surface microtopographic data using 3-D stylus profilometry and to display the data as intensity variations on a television monitor is described. Images of the data are generated from an array of 512 by 512, 8 bit digitized surface height values. The surface slope and wavelength capabilities of stylus instruments are compared with other surface microtopography measurement techniques to highlight their unique high vertical resolution capabilities for low sloped surfaces. Finally, examples of some alternative means for displaying 3-D data sets are given for three types of surface irregularities; a discrete feature, a periodic profile surface, and a random profile surface. These representations of the topography are also compared with scanning electron micrographs of the same surface irregularities.

501,221
PB85-205854 Not available NTIS
 National Bureau of Standards, Gaithersburg, MD.
Look at the Electronic Analytical Balance.
 Final rept.,
 M. Schoonover. 1980, 8p
 Pub. in Analytical Chemistry 54, n8 p973-980 1982.

Keywords: *Weight indicators, *Electric equipment, Measuring instruments, Weight(Mass), Performance evaluation, Reprints.

Today electronic balances are being used for everything from counting batches of resistors to adjusting the component ratio of epoxy mixtures. Many of these balances are suitable for the most demanding analytical work while others are less precise but serve many purposes well. The paper describes the general principles of the modern electronic analytical balance.

501,222
PB85-206704
 (Order as PB85-206324, PC A13/MF A01)
 Rockwell International, Thousand Oaks, CA. Science Center.
Diffuse Multilayer Analysis Using a Multiflux Method.
 S. O. Sari. Apr 85, 4p
 Included in OM85: Basic Properties of Optical Materials. Summaries of Papers, p154-157 Apr 85.

Keywords: *Optical materials, *Optical coatings, *Coatings, Light scattering, Maxwells equations.

The use of uniform material layers to form multilayer films forms the basis for an extensive coating technology. The transmissive and reflective properties of such structures are dominated by optical interference occurring among the layers. Comparatively less attention seems to have been given to treating stratified media consisting of random rather than uniform material layers. Within such structures, the optical scattering properties of each sublayer dominate the optical properties. Some previous work on diffuse coatings has been concerned with investigations of surface-roughened layers and the form of diffuse scattering from one or more roughened interfaces. Such analytical investigations have been based on lowest-order solutions to Maxwell's equations at a perturbed roughened interface, a calculational procedure which has been carried out by several different authors in recent years. The present objective is to point toward a possible alternative method for treating diffuse scattering. Examples would include aggregate suspensions, artificial dielectrics, solids containing scattering defects, paint layers or inhomogeneous recording materials. This analysis may have applications to optical material studies such as ensemble microparticle drop sizing or other related topics of current interest. It may serve as an adjunct to scattering models based on direct solutions to Maxwell's equations for various scattering geometries.

501,223
PB85-207033 Not available NTIS
 National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div.
Characterization of a Standard Reference Superconductor for Critical Current and a Summary of Other Standard Research at NBS (National Bureau of Standards).
 Final rept.,
 A. F. Clark, and L. F. Goodrich. 1984, 5p
 Sponsored by Department of Energy, Washington, DC. Office of Fusion Energy.
 Pub. in Proceedings of Int. Cryogenic Engineering Conf. (10th), Helsinki, Finland, July 31-August 3, 1984, p433-437.

Keywords: *Calibrating, *Standards, *Standard reference materials, *Critical current, Niobium tin.

A standard reference material can be useful for the calibration of measurement apparatus and interlaboratory comparison of research results. The authors have carefully characterized the first practical superconductor SRM for critical current and it is now available from NBS as 'Standard Reference Material 1457 Superconducting Critical Current - NbTi Wire.' The selection, characterization, and statistical analysis of this material are described. The progress in other standards research will also be discussed for large conductor critical current, ac losses, stability, and critical field.

501,224
PB85-207090 Not available NTIS
 National Bureau of Standards, Gaithersburg, MD. Inorganic Materials Div.
Interferometric High Pressure Gauge for the Diamond Anvil Cell Useful at High Temperatures.
 Final rept.,
 J. A. H. da Jornada, S. Block, and G. J. Piermarini. 15 Sep 84, 3p
 Sponsored by Conselho Nacional de Pesquisas, Rio de Janeiro (Brazil) and Universidade Federal do Rio Grande do Sul, Porto Alegre (Brazil). Inst. de Fisica. Pub. in Applied Physics Letters 45, n6 p700-702, 15 Sep 84.

Keywords: *Pressure gages, High temperature tests, Optical interferometers, Pressure measurement, Reprints, *Anvil cells, Zinc tungstates, Refractive index.

A new method of precise pressure measurement in the diamond anvil cell, especially useful at high temperatures, is presented. It is based on the measurement of the channelled spectrum of a miniature Fabry-Perot etalon interferometer placed inside the cell. The validity of the method has been verified with an interferometric gauge of ZnWO₄.

501,225
PB85-207157 Not available NTIS
 National Bureau of Standards, Gaithersburg, MD.
Picosecond Streak Camera Fluorometry: A Review.
 Final rept.,
 A. J. Campillo, and S. L. Shapiro. 1983, 19p
 Pub. in IEEE (Institute of Electrical and Electronics Engineers) Jnl. of Quantum Electronics QE-19, n4 p585-603 Apr 83.

Keywords: *Laboratory equipment, *Fluorometers, Reviews, Fluorescence, Design criteria, Performance evaluation, Chemical analysis, Reprints, *Picosecond pulses.

A general tutorial survey is presented describing the use of ultrafast streak cameras in picosecond fluorometry. Current instruments exhibit time resolutions of 1 to 10 ps with detection sensitivities of a few photoelectrons. When linear photoelectric recording is employed, a real-time direct display of optical transients is provided. Representative examples from the literature in physics, chemistry, and biology are given as well as an extensive bibliography.

501,226
PB85-207215 Not available NTIS
 National Bureau of Standards, Gaithersburg, MD.
Temperature and Thermometry.
 Final rept.,
 B. W. Mangum. 1985, 9p
 Pub. in Encyclopedia of Physics, p1215-1223 1985.

Keywords: *Temperature measurement, *Temperature measuring instruments, Performance evaluation, Reprints, *Thermometry.

The report gives a very brief history and discussion of thermometry and temperature scales. The fundamental bases of temperature scales and some of the most commonly used thermometers are briefly discussed.

501,227
PB85-207421 Not available NTIS
 National Bureau of Standards (NEL), Gaithersburg, MD. Electrosystems Div.
Measurement of Net Space Charge Density Using Air Filtration Methods.
 Final rept.,
 R. H. McKnight. Apr 85, 6p
 Sponsored by Department of Energy, Washington, DC.

Field 14—METHODS AND EQUIPMENT

Group 14B—Laboratories, Test Facilities, and Test Equipment

Pub. in IEEE (Institute of Electrical and Electronics Engineers) Transactions on Power Apparatus and Systems PAS-104, n4 p971-976 Apr 85.

Keywords: *Space charge, Measurement, Filtration, Air flow, Density(Number/volume), Reprints.

The efficiency of a high efficiency particulate air (HEPA) or absolute filter for removing charge from an air stream has been measured for a variety of space charge and air flow conditions. Ion densities ranged from 100,000 to 1,000,000/cu cm and were for positive and negative space charge as well as mixtures. The space charge was made up predominantly of ions with mobilities greater than 0.00001 sq m/Vs. For all conditions studied, the transmission of the filter was less than 0.1%. For space charge consisting of ions of one polarity, space charge density measurements made using HEPA filters and ion counters may be compared directly. The filter is well suited for accurate measurements of net space charge density.

501,228
PB85-208031 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Optical Test Method for Measuring Biaxial Deformations.
Final rept.,
R. S. Polvani, C. P. Reeve, and R. C. Veal. Jan 85, 5p
Contract N00014-82-F-0038
Pub. in Jnl. of Testing and Evaluation 13, n1 p69-73 Jan 85.

Keywords: *Deformation, *Optical measurement, Extensometers, Beryllium, Tests, Reprints.

A new and simple method is described for the measurement of biaxial deformation with a resolution of 0.025 micrometer (1 microinch). The basis for this technique is the use of an optical extensometer.

501,229
PB85-208064 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymer Science and Standards Div.
Some Remarks on the History and Development of the ASTM Committee E-37 Purity Method.
Final rept.,
C. M. Guttman. 1984, 6p
Pub. in American Society for Testing and Materials, Special Technical Publication 838, p16-21 1984.

Keywords: *Purification, *Standards, *Materials tests, Sampling, Performance evaluation, Reprints.

The history and development of the ASTM Committee E-37 Purity Method are discussed. The early protocols and resulting round robin data are considered. The importance of the development of suitable sample materials to be used by the task group members in parallel with the methods development will also be discussed.

501,230
PB85-208106 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Semiconductor Materials and Processes Div.
Comparison of Depth Profiling of (10)B in Silicon Using Spreading Resistance Profiling, Secondary Ion Mass Spectrometry, and Neutron Depth Profiling.
Final rept.,
J. R. Ehrstein, R. G. Downing, B. R. Stallard, D. S. Simons, and R. F. Fleming. 1984, 15p
Pub. in American Society for Testing and Materials, Special Technical Publication 850, p409-425 Oct 84.

Keywords: *Silicon, *Semiconductor doping, Reprints, *Boron 10, *Ion implantation, Secondary ion mass spectroscopy, Spreading resistance.

Depth profiling of intentional dopants is an important measurement in the semiconductor industry both for process and device modeling and for process control. A comparison of (10)B implants into silicon as measured by Spreading Resistance Profiling (SRP), Secondary Ion Mass Spectrometry (SIMS) and by Neutron Depth Profiling (NDP) is presented. The boron implantations were done at several fluences and energies into bare silicon and through several thicknesses of thermally grown oxides. Sources of error and their relation to observed differences among the techniques will be discussed.

501,231
PB85-222107 Not available NTIS

National Bureau of Standards, Gaithersburg, MD. Polymers Div.

Measurement of a Piezoelectric delta Constant for Poly(Vinylidene Fluoride) Transducers Using Pressure Pulses.
Final rept.,

A. J. Bur, and S. C. Roth. 1 Jan 85, 6p
Sponsored by Air Force Armament Lab., Eglin AFB, FL.
Pub. in Jnl. of Applied Physics 57, n1 p113-118, 1 Jan 85.

Keywords: *Transducers, Piezoelectricity, Measurement, Vinylidene chloride resins, Reprints.

The hydrostatic piezoelectric coefficient $d_{sub h}$ has been measured for biaxially-oriented poly(vinylidene fluoride) transducers using pressure pulses having peak values of 1.8×10 to the 7th power Pa (2600 psi) and a pulse width of approximately 10 ms. For these measurements, the sample was placed in an oil pressure chamber at room temperature and the pressure pulse was initiated by dropping a 16-kg mass onto a plunger in the chamber. Since adiabatic compressional heating accompanies the pressure pulse, temperature compensation of the transducer was necessary. This was achieved by incorporating a thermocouple in the bilaminate configuration of the transducer and by amplifying the thermocouple signal appropriately to account for the pyroelectric response due to adiabatic heating, which was approximately 15% of the transducer signal. The calculation of $d_{sub h}$ shows that the response of the bilaminate transducer is linear up to 1.8×10 to the 7th power Pa (2600 psi).

501,232
PB85-224418 PC A04/MF A01
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Building Technology.
Performance Requirements and Preliminary Design of a Boundary Layer Wind Tunnel Facility.
Final rept.,
R. D. Marshall. May 85, 68p NBSIR-85/3168

Keywords: *Wind tunnels, *Boundary layer, Test facilities, Design, Performance, Contraction, Diffusers, Aerodynamics, Buildings, Structures, *Wind engineering.

This report describes performance characteristics and design details of a boundary layer wind tunnel for supporting research activities within the Center for Building Technology. Two preliminary designs, the first consisting of a conventional closed-circuit scheme in an over/under configuration and the second consisting of an open-circuit scheme with a 'pusher' or 'blow-down' configuration, are addressed.

501,233
PB85-227668 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Applied Mathematics.
Subharmonic Frequency Locking in the Resistive Josephson Thermometer.
Final rept.,
M. van Veldhuizen, and H. A. Fowler. 1 May 85, 6p
Pub. in Physical Review B 31, n9 p5805-5810, 1 May 85.

Keywords: *Temperature measuring instruments, Josephson junctions, Electrical impedance, Cryogenics, Reprints, *Thermometers, SQUID devices.

Phase-locked oscillatory solutions are examined as a basis for the dc impedance of the resistive superconducting quantum-interference device Josephson thermometer. The calculations are based on the resistively shunted junction model in the limit $2\pi(L_{sub s})(I_{sub c})/(\Phi_{sub 0}) = \text{or} > 1$, where $(L_{sub s})$ is the loop inductance and $(I_{sub c})$ is the junction critical current, and for a junction resistance large compared with the external shunt resistance. An algorithm for representing frequency entrainment in (κ, ω) space (drive amplitude, frequency) leads to zones with rotation number p/q having the form of leaf-shaped regions joined and overlapping at their tips. High-resonance zones are very thin and locally similar. No chaotic behavior has been observed. The model can simulate the 'rising' curves of dc impedance as a function of drive amplitude.

501,234
PB85-229441 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.

Automated Apparatus for X-ray Pole Figure Studies of Polymers.

Final rept.,
J. D. Barnes, and E. S. Clark. 1985, 8p
Pub. in Proceedings of the ACS (American Chemical Society) Division of Polymeric Materials: Science and Engineering, Miami Beach, Florida, v52 p382-388 Apr 85.

Keywords: *Automatic control equipment, *X ray diffraction, *Polymers, *Crystal structure, Laboratory equipment, Fortran, Computer programs, Performance evaluation, Design criteria, Crystallite, Computer applications.

The authors have adapted a commercially available x-ray diffractometer normally used for structure determinations on single crystals to operate as a very flexible device for performing x-ray pole figure determinations and related studies on polymeric materials. Descriptions of crystallite orientations, as provided by pole figures, are useful in studying many aspects of the behavior of products made from semicrystalline polymers. The paper describes the software that they have written for their pole figure facility. Except for some vendor-provided routines to drive the hardware interface all of their software is written in FORTRAN. Menu driven operation is provided to maximize user convenience.

501,235
PB85-229458 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.
Software for Liquid Size Exclusion Chromatography Data Collection and Analysis.
Final rept.,

J. D. Barnes, B. Dickens, and F. L. McCrackin. 1985, 9p
Pub. in Proceedings of the ACS (American Chemical Society) Division of Polymeric Materials: Science and Engineering, Miami Beach, Florida, v52 p291-298 Apr 85.

Keywords: *Chromatographic analysis, *Operating systems(Computers), *Data processing, Fortran, Molecular weights, Automation, Laboratories, *Liquid size exclusion chromatography, *Computer software, *Applications programs(Computers), *Computer aided analysis, Computer applications.

The paper describes software that is used for data collection and analysis from a size-exclusion liquid chromatograph. The chromatograph is a commercially available instrument that provides on board microprocessor control of the specimen injection functions. The authors use a commercially available microcomputer as a passive listener connected to the chromatograph output to collect, store, and analyze the data. The data collection and analysis software is written in FORTRAN. Maximum use is made of graphical displays to aid the user's judgement in interpreting the data. All operations are menu driven, so that the user does not need to be familiar with the computer's operating system. Data archiving functions are built in to facilitate after-the-fact retrieval of the data.

501,236
PB85-229896 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Mechanical Production Metrology Div.
Deconvolution by Design - An Approach to the Inverse Problem of Ultrasonic Testing.
Final rept.,

D. Eitzen, N. Hsu, A. Carasso, and T. Proctor. 1985, 10p
Pub. in the Review of Progress in Quantitative Nondestructive Evaluation, v4A p179-188 1985.

Keywords: *Nondestructive tests, *Ultrasonic tests, *Deconvolution, Inverse problems.

In the paper the authors present some preliminary results on a new approach to the problem of characterizing flaws using ultrasonics. The approach takes advantage of the fact that they have control over the time waveform of the probing pulse in an ultrasonic test. It also takes advantage of some special properties of the inverse Gaussian function and an effective, stable, continuous deconvolution procedure which is based on the special function. The procedure also has the special feature that the error in the resultant of the deconvolution, which contains all available information about the flaw-scatterer, can be estimated in a powerful way. First they present the problem formulation and

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the analytical reasoning. They then discuss the inverse Gaussian function, the deconvolution procedure based on the probe function, and point out some of the special features of the probe function and the procedure. They also present some numerical tests and results using the procedure, demonstrate that the tools necessary to implement the procedure are within grasp, and present some preliminary experimental results.

501,237
PB85-230027 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Semiconductor Materials and Processes Div.
Optical Linewidth Measurement on Patterned Metal Layers.
Final rept.,
D. Nyssonen. 1984, 7p
Pub. in SPIE 480, p65-70 1984.

Keywords: *Line width, Optical measurement, Lithography, Integrated circuits, Wafers, Reprints.

In a previous paper, a waveguide model was developed for the imaging of micrometer-sized lines patterned in thick layers of dielectric materials (silicon dioxide) with application to linewidth measurement on integrated-circuit wafers. The paper describes the extension of this work to metals characterized by their complex index of refraction, $n + iK$, as well as the inclusion of a sublayer such as a silicon dioxide insulating layer. This extension allows the modeling of optical imaging and linewidth measurement on metal-on-silicon (MOS) structures. It is shown that the image structure for metals at and near focus is different from that for dielectrics. Thick and thin layer (less than 200 nm) imaging is compared. Experimental image profiles of metal lines at and near focus are also shown. The experimental data were obtained from a bright-field microscope using a laser source (530 nm) and controlled spatial coherence.

501,238
PB85-230381 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Semiconductor Materials and Processes Div.
National Bureau of Standards, a Review of NBS's Activities in the Area of Linewidth Measurement.
Final rept.,
D. Nyssonen. 1984, 8p
Pub. in Proceedings of the Scientific Apparatus Makers Association, The Future of Optical Technologies in the Semiconductor Industry, Sunnyvale, California, May 23, 1983, p1-7 Mar 84.

Keywords: *Line width, *Measurement, Optical measurement, Calibrating, Standard reference materials.

The manuscript is a summary of a talk covering current NBS activities in linewidth measurement including research, calibration of standard reference materials (SRMs), development of calibration procedures and test methods, and technology transfer. The current status of photomask linewidth SRMs is discussed (anti-reflective 'gold' chromium SRMs 474 and 475, bright chromium SRM 476, and the 3X reticle SRM 1830). Wafer linewidth measurements are divided into two categories, thin layers (less than approximately 200 nm) and thick layers. The design of the linewidth standard for thin layers is described. Research problems remaining for thick layers are described along with current NBS waveguide modeling. Instrumentation used for both photomask and wafer calibrations is also described. NBS plans for development of SEM/e-beam instrumentation and SRMs are also included.

501,239
PB85-230795 Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Time and Frequency Div.
Frequency Measurements from the Microwave to the Visible, the Speed of Light, and the Redefinition of the Meter.
Final rept.,
K. M. Evenson. 1983, 28p
Pub. in Proceedings of the North Atlantic Treaty Organization Advanced Study Institute on Quantum Metrology and Fundamental Physical Constants, Erice, Italy, November 16-28, 1981, NATO ASI Series B: Physics, v98 p181-207 1983.

Keywords: *Frequency measurement, *Length, *Metrology, *Standards, *Light speed, *Meter, Laser radiation.

The techniques of laser frequency measurement, especially those leading to the measurements of the frequency of visible light, are described. The use of these techniques has led to much higher accuracy in spectral measurements, a hundred-fold increase in the accuracy of the value of the speed of light, and to a proposed redefinition of the meter, fixing the value of the speed of light. The use of stabilized lasers in these measurements, some of the characteristics of the metal-insulator-metal diode used in high speed detection, and the realization of the meter with the proposed new definition are described.

501,240
PB85-230878 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.
Polymer Pressure Gage for Dynamic Pressure Measurements.
Final rept.,
A. J. Bur, and S. C. Roth. 1985, 6p
Pub. in Proceedings of the Symposium on Interaction of Non-Nuclear Munitions with Structures (2nd), Panama City, Florida, April 15-18, 1985, p291-295.

Keywords: *Pressure gages, Thin films, Polyvinyl fluoride, Pressure sensors.

The pressure sensing element of this transducer is a thin film of polyvinylidene fluoride. The transducer is designed to measure dynamic pressures in the presence of thermal pulses which are produced by adiabatic compressional heating of the PVDF and its surroundings. Adiabatic heating of the PVDF will reduce its charge output by a constant 8%. Adiabatic heating of the surroundings will vary with each environment. Two approaches to compensating for environmental compressional heating are used.

501,241
PB85-236354 PC A03/MF A01
National Bureau of Standards, Gaithersburg, MD. Public Information Div.
NBS (National Bureau of Standards) Research Reports, July 1985.
Special pub.
Jul 85, 38p NBS/SP-680/3
See also PB85-127421. Library of Congress catalog card no. 85-600549.

Keywords: *Research projects, Industries, Composite materials, Fire tests, Buildings, Heat pumps, Ozone, Electric current, Standards, Ultraviolet radiation, Calibrating, Astronomical telescopes, Quality assurance, Clinical chemistry, *National Bureau of Standards.

Contents:
NBS research on polymer composites:
laying the scientific foundation for industrial advance;
Searching for the more vital volt, the apter ampere;
Evaluating volts, jolts, and lightning bolts:
all in a day's work at NBS;
NBS fire research is framework for safer buildings;
The making of the advanced heat pump:
research to influence the marketplace;
Measuring the two 'personalities' of ozone;
New ultraviolet wavelength standards will aid astronomy;
Calibrations for the space telescope;
NBS program boosts quality of clinical measurements.

501,242
PB85-237352 (Order as PB85-237329, PC A04/MF A01)
National Bureau of Standards (NEL), Boulder, CO. Chemical Engineering Science Div.
High Temperature, High Pressure Reaction-Screening Apparatus.
T. J. Bruno, and G. L. Hume. 7 Jan 85, 3p
Included in Jnl. of Research of the National Bureau of Standards, v90 n3 p255-257 May-Jun 85.

Keywords: *High temperature tests, *High pressure tests, *Decomposition reactions, *Laboratory equipment, *Fluids, Design criteria, Performance evaluation, Mixtures, Phase transformation, Gas chromatography, Sampling, Chemical properties, Chemical equilibrium, PVT properties.

This short note describes an apparatus that has been designed and constructed to allow assessment of the extent of chemical decomposition of fluids and fluid mixtures under high temperature, high pressure conditions. The apparatus is used to screen fluid systems

prior to PVT (pressure-volume-temperature) or VLE (vapor-liquid equilibrium) experiments under severe conditions. For a predetermined residence time, the fluids are maintained at the temperature and pressure at which the PVT or VLE experiment will be conducted. The residence time in the reactor is comparable to the expected residence time in the PVT or VLE apparatus. Samples of fluid are withdrawn directly at regular intervals for analysis by gas chromatography, or collected in a sampling vessel for more extensive analysis.

501,243
PB85-239218 PC A04/MF A01
National Bureau of Standards, Gaithersburg, MD. Office of Product Standards Policy.
NVLAP (National Voluntary Laboratory Accreditation Program) Director of Accredited Laboratories Midyear Update.
H. W. Berger. Jul 85, 53p NBSIR-85/3204

Keywords: *Directories, *Laboratories, Sites, Projects, Test facilities, Tests, *Accreditation, *National Voluntary Laboratory Accreditation Program.

The directory is an update of the 1984 NVLAP Directory of Accredited Laboratories. It provides information on the activities of the National Bureau of Standards in administering the National Voluntary Laboratory Accreditation Program (NVLAP) during calendar year 1985. The status of current programs is briefly described and a summary of laboratory participation is provided. All accredited laboratories are listed along with the test methods for which they are accredited. Four Indexes cross reference the laboratories by name, NVLAP Lab Code Number, test method, accreditation program, and geographical location.

501,244
PB85-242162 PC A03/MF A01
National Bureau of Standards, Gaithersburg, MD. Office of Product Standards Policy.
Acoustics LAP (Laboratory Accreditation Program) Handbook. Operational and Technical Requirements of the Laboratory Accreditation Program for Acoustical Testing Services.
R. L. Gladhill, W. A. Hall, J. Horlick, and H. W. Berger. Jul 85, 32p NBSIR-85/3199

Keywords: *Laboratories, Acoustics, Requirements, Accreditation.

The document explains the operational and technical requirements of the Laboratory Accreditation Program (LAP) for Acoustics (Acoustics LAP). All of the steps leading to accreditation are discussed. Technical requirements are explained indicating how the NVLAP criteria are applied. It is intended for use by staff of accredited laboratories, those seeking accreditation, other laboratory accreditation systems, and others needing information on the requirements for NVLAP accreditation under this LAP.

501,245
PB85-244069 PC A03/MF A01
National Bureau of Standards, Gaithersburg, MD. Office of Nondestructive Evaluation.
NDE (Non-Destructive Evaluation) Publications, 1982.
L. Mordfin. Jun 85, 37p NBSIR-85/3183
See also PB83-184622.

Keywords: *Nondestructive tests, *Bibliographies, Abstracts, National Bureau of Standards.

This is the sixth in a series of bibliographies of NBS publications on nondestructive evaluation (NDE). It provides bibliographic citations, with selected abstracts, for 124 publications that appeared in the open literature, primarily during calendar year 1982. A detailed subject index is included as well as information on how copies of many of the publications may be obtained.

501,246
PB86-101920 Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Time and Frequency Div.
Laser-Cooled-Atomic Frequency Standard.
Final rept.,
J. J. Bollinger, J. D. Prestage, W. M. Itano, and D. J. Wineland. 1985, 4p
Sponsored by Air Force Office of Scientific Research, Bolling AFB, DC., and Office of Naval Research, Arlington, VA.

Field 14—METHODS AND EQUIPMENT

Group 14B—Laboratories, Test Facilities, and Test Equipment

Pub. in Physical Review Letters 54, n10 p1000-1003, 11 Mar 85.

Keywords: *Frequency standards, *Atomic clocks, Reprints, Laser cooling, Penning traps, Beryllium ions, Beryllium 9.

The first frequency standard based on laser-cooled atoms is reported. Beryllium atomic ions were stored in a Penning trap and cooled by radiation pressure from a laser. The frequency of the 9Be^+ (MI,MJ) $= (-3/2, +1/2) \leftrightarrow (-1/2, +1/2)$ ground-state hyperfine transition at its magnetic-field-independent point was determined to be 303016377.265070(57) Hz. The accuracy of a frequency standard referenced to this transition was comparable to the best frequency standards, which are based on cesium atomic beams.

501,247

PB86-102241 PC A03/MF A01
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Mfg. Engineering.
Sizing of Polystyrene Spheres Produced in Microgravity,
G. Mulholland, G. Hembree, and A. Hartman. Jul 85, 26p NBSIR-84/2914

Keywords: *Latex, *Polystyrene, *Spheres, *Size determination, Standard deviation, Weightlessness, *Space manufacturing, Space shuttles, Transmission electron microscopy.

The standard deviation of the size distribution was determined for a polystyrene latex produced in a space shuttle experiment and in an earth-bound control experiment. Values determined from direct measurement of transmission electron micrographs, corrected for magnification distortion, were 0.035 micrometer for the space grown material and 0.15 micrometer for the control. The standard deviations obtained from an aerodynamic particle sizer were only slightly greater than those obtained by TEM; 0.042 micrometer and 0.20 micrometer for the shuttle and ground material respectively. However these values were produced in a few hours versus the several weeks it took for the electron microscopy. Both of the techniques used here resulted in measured standard deviations significantly smaller than those previously reported for this material.

501,248

PB86-103454 PC A06/MF A01
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.
Response Behavior of Hot-Wires and Films to Flows of Different Gases,
W. M. Pitts, and B. J. McCaffrey. Jul 85, 124p
NBSIR-85/3203
Sponsored by Air Force Office of Scientific Research, Bolling AFB, DC.

Keywords: *Flow measurement, Hot wire anemometers, Gas flow, Velocity measurement, Reynolds number, Nusselt number, Heat transfer, Correlations, Cylindrical bodies, Convection, Vortices, Calibrating, Hot-film anemometers, Accommodation coefficient.

Measurements of the voltage output for hot-wire and film anemometers placed in flows of nine different gases have been made as a function of flow velocity. In order to obtain these correlations it has been necessary to consider and correct for the effects of probe end conduction losses, temperature dependencies of gas molecular properties, flow slip at the probe surfaces, and gas accommodation. The importance of the nature of the flow over the cylindrical devices to the heat transfer behavior is described. A previously unreported hysteresis in the heat transfer behavior for RE 44 has been characterized and attributed to the presence or absence of eddy shedding from the heated cylinder.

501,249

PB86-106747 PC A04/MF A01
National Bureau of Standards (NML), Gaithersburg, MD. Office of Standard Reference Materials.
Feasibility Study for the Development of Standards Using Differential Scanning Calorimetry.
Final rept.,
J. E. Callanan, S. A. Sullivan, and D. F. Vecchia. Aug 85, 59p NBS/SP-260/99
Also available from Sup. of Docs as SN003-003-02675-1. Library of Congress catalog card no. 85-600567.

Keywords: Feasibility, Standards, Calibrating, Materials tests, Temperature, Heat flow, Enthalpy, *Standard reference materials, *Differential scanning calorimetry.

The tremendous increase in the use of differential scanning calorimetry, coupled with the decrease in the capability for conventional precision calorimetry, has created a need for more and better thermal standards for use with scanning calorimeters and other thermal instruments currently available, such as thermomechanical analyzers. The development of these standards by methods such as adiabatic or drop calorimetry is impractical because of the number and variety of standards required, the associated expense, and the lack of facilities and personnel to do the certification. A two-part study was designed to evaluate the capability of a differential scanning calorimeter for developing temperature and enthalpy of fusion standards. Part I evaluated the variability of the differential scanning calorimeter (DSC) and factors which affected it; Part II applied American Society of Testing Materials (ASTM) procedures for the temperature and heat flow calibration. The study shows that fusion standards can be developed with a differential scanning calorimeter.

501,250

PB86-108180 PC A05/MF A01
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Building Technology.
Assessment of the NBS (National Bureau of Standards) 1-Meter Guarded-Hot-Plate Limits.
Final rept.,
B. G. Rennex. Aug 85, 98p NBSIR-85/3221
Contract DE-AI05-85OR21513
Sponsored by Department of Energy, Washington, DC. Office of Buildings Energy R and D.

Keywords: *Thermal insulation, Thermal resistance, Thermal conductivity, Performance evaluation, Calibrating, *Guarded hot plates, *Building materials.

Accurate measurement of the thermal resistance of insulation and building materials is a matter of national interest. A viable national calibration program must consist of accurate apparatuses, appropriate test methods, and calibration specimens available over the needed ranges of test and material parameters, such as temperature and apparent thermal conductivity. The apparatuses are operated according to the test methods to provide these calibration specimens. It is necessary to know the apparatus accuracy over the entirety of the operating ranges over which the calibration specimens are measured. The objective of this report is to evaluate the operating capability of the NBS 1-m Guarded-Hot-Plate apparatus according to three kinds of limiting factors. The first kind is the limits of temperature over which the various apparatus components can be used without suffering damage. The second kind is the limits of plate temperatures, specimen thickness, atmospheric pressure, and relative humidity that can be achieved with the existing control systems. The third kind is any limits on the values of apparent thermal conductivity, thermal resistance, or specimen thickness due to measurement error considerations.

501,251

PB86-110103 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Building Equipment Div.
Humidity Sensors for HVAC (Heating, Ventilation and Air-Conditioning) Applications.
Final rept.,
C. W. Hurley, and S. Hasegawa. May 85, 18p
Sponsored by Civil Engineering Lab. (Navy), Port Hueneme, CA.
Pub. in Proceedings of International Symposium on Recent Advances in Control and Operation of Building HVAC Systems, Trondheim, Norway, May 22-23, 1985, p173-190.

Keywords: *Moisture content, *Environmental engineering, *Psychrometers, *Dew point, *Buildings, Hygrometers, Heating equipment, Ventilation, Air conditioning, Cost analysis, Ideal gas law.

The monitoring and control of the moisture content of the air within a building is required to operate the heating, ventilation and air-conditioning (HVAC) equipment in the most efficient manner to meet the demands of the people and equipment working in the building. The ideal gas equation can be used for this purpose since only negligible errors will result. Seven types of relative humidity sensors are discussed. The basic principles of operation, cost ranges, expected accuracies, linearities, operating limits, etc. are given. A section is devoted to methods of avoiding the high limits of relative humidity sensors. Finally, a discussion of the principles of operation, cost, operating limits, etc. is presented on dew-point hygrometers and their applications in HVAC systems.

501,252

PB86-111374 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Gas and Particulate Science Div.
Characteristics of Backscattered Electron Detectors for Scanning Electron Microscopy.
Final rept.,
D. E. Newbury. 1981, 8p
Pub. in Proceedings of Annual Conference on Microbeam Analysis Society (16th), Vail, CO., July 13-17, 1981, p1-8.

Keywords: Electron scattering, Backscattering, Scintillation counters, Solid state counters, *Scanning electron microscopy, *Electron detection, *Electron counters.

The backscattered electron signal in the scanning electron microscope carries useful contrast information on atomic number differences, topography, crystallography, and magnetism in a sample. Detectors for backscattered electrons fall into four categories (1) scintillators; (2) backscattered to secondary conversion with detection with a scintillator; (3) solid state diodes; and (4) specimen current. Important detector properties include: (1) solid angle of collection; (2) take-off (emergence) angle; (3) energy-response; (4) frequency response; and (5) sensitivity to electron trajectory effects. These properties are compared for the various detectors.

501,253

PB86-111770 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD.
Impedance Changes Produced by a Crack in a Plane Surface.
Final rept.,
A. H. Kahn. 1982, 5p
Pub. in Proceedings of the Air Force/Defense Advanced Research Projects Agency Symposium (8th), Boulder, CO., August 2-7, 1981. Review of Progress in Quantitative Nondestructive Evaluation, v1 p369-373 1982.

Keywords: *Eddy current tests, Cracking(Fracturing).

A report will be presented of calculations of eddy currents in the vicinity of a crack in a plane slab of conducting material. The exciting field is taken as uniform and parallel to the slab and the plane of the crack. In these calculations, the crack depth is arbitrary, as is its inclination to the plane of the slab. The eddy current problem was solved by a boundary integral equation method (also known as the boundary element method). The induced currents at the surface of the conductor and on the crack will be shown for selected crack depths representative of all ranges of the ratio of crack depth to the electromagnetic skin depth, and for selected angles of crack inclination. The total impedance change produced by the crack will be given for arbitrary crack depth and inclination.

501,254

PB86-112059 Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Time and Frequency Div.
Trapped Ions, Laser Cooling, and Better Clocks.
Final rept.,
D. J. Wineland. Oct 84, 6p
Pub. in Science 226, p395-400, 26 Oct 84.

Keywords: *Atomic clocks, *Frequency standards, *Atomic spectroscopy, Reprints, *Laser cooling, *Ion traps, Laser spectroscopy.

Ions that are stored in electromagnetic 'traps' provide the basis for extremely high resolution spectroscopy. By using lasers, the kinetic energy of the ions can be cooled to millikelvin temperatures, thereby suppressing Doppler frequency shifts. Potential accuracies of frequency standards and clocks based on such experiments are anticipated to be better than one part in 10 to the 15th power.

501,255

PB86-112067 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Organic Analytical Research Div.

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Factors Affecting the Reversed-Phase Liquid Chromatographic Separation of Polycyclic Aromatic Hydrocarbon Isomers.

Final rept.,
S. A. Wise, and L. C. Sander. May 85, 8p
Pub. in Jnl. of High Resolution Chromatography and Chromatography Communications 8, p248-255 May 85.

Keywords: *Aromatic polycyclic hydrocarbons, *Chemical analysis, *Chromatographic analysis, Separation, Mathematical models, Polymers, Reprints, *Reversed phase liquid chromatography, Monomers.

Reversed-phase liquid chromatography (LC) on C18 stationary phases provides excellent selectivity for the separation of polycyclic aromatic hydrocarbons (PAH). Recent studies have shown that several factors affect selectivity for the LC separation of PAH including phase type (monomeric or polymeric), pore diameter and surface area of the silica substrate, and surface density of the C18 ligands. In this paper the separation of eleven PAH isomers of molecular weight 278 is used to further illustrate the effect of stationary phase characteristics and shape of the solute (length-to-breadth ratio, L/B) on retention and selectivity. Based on these studies, a model is proposed to describe the retention of PAH on polymeric C18 phases.

501,256

PB86-112075 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Semiconductor Devices and Circuits Div.
Electrical Test Structure for Proximity Effects Measurement and Correction.

Final rept.,
D. Yen, L. W. Linholm, and W. B. Glendinning. Jul 85, 4p
Pub. in Jnl. of the Electrochemical Society 132, n7 p1726-1729 Jul 85.

Keywords: *Test specimens, *Electronic test equipment, *Lithography, Design criteria, Distance, Experimental designs, Reprints, Electron beam lithography.

The paper describes the design of a proximity effect test structure and electrical test method for estimating the magnitude of proximity effects in electron-beam lithography. The test structure consists of a van der Pauw cross resistor for measuring sheet resistance, a bridge resistor for measuring electrical linewidth, and a second bridge resistor simulating a close line-space environment for measuring electrical linewidth where proximity exposure effects from nearby patterns may be encountered. In this experiment, test structures were delineated in aluminum on silicon wafers using electron-beam exposure and wet chemical etching. Electrical measurements from these test structures are compared to optical measurements to verify the measurement method. In addition, results from the test structures are used to estimate the parameters for the gaussian model commonly used for proximity correction.

501,257

PB86-112190 Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div.
Technique for Extending the Dynamic Range of the Dual Six-Port Network Analyzer.

Final rept.,
J. R. Juroshek, and C. A. Hoer. Jun 85, 7p
Sponsored by Aerospace Guidance and Metrology Center, Newark AFS, OH.
Pub. in IEEE (Institute of Electrical and Electronics Engineers) Transactions on Microwave Theory and Techniques, MTT-33 n6 p453-459 Jun 85.

Keywords: *Network analyzers, Microwave equipment.

The dynamic range of the six-port type of automatic network analyzer is typically limited to measuring two-port devices with a transmission coefficient in the range of 0 to -60 dB. The following describes a subcarrier approach for extending the dynamic range of the dual six-port network analyzer.

501,258

PB86-112737 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Office of Standard Reference Materials.

Role of NBS SRM's (National Bureau of Standards Standard Reference Materials) in Quality Assurance.

Final rept.,
S. D. Rasberry. 1983, 6p
Sponsored by American Society for Quality Control, Inc., Milwaukee, WI.
Pub. in Proceedings of Annual American Society Quality Control Transactions (37th), Boston, MA., May 24-26, 1983, p343-348.

Keywords: *Quality assurance, Quality control, Measurement, Accuracy, *Standard reference materials, Traceability.

Requirements for 'traceability to NBS' can be found in a variety of regulations and standards. As the agencies requiring traceability do not necessarily define or interpret these requirements uniformly, confusion concerning compliance with such requirements is not uncommon. This paper and a companion paper on NBS Calibration Services discusses the traceability issue from NBS' perspective. Statistical quality control techniques developed originally for industrial production processes can be employed to ensure accurate measurements on a continuing basis using either Standard Reference Materials or calibration services where they are available from NBS.

501,259

PB86-112794 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Building Physics Div.

Design of Round-Robin Tests Using Guarded/Calibrated Hot Boxes, Guarded Hot Plates, Heat Flow Meters.

Final rept.,
F. J. Powell, and E. L. Bales. 1983, 17p
Sponsored by American Society for Testing and Materials, Philadelphia, PA., and Oak Ridge National Lab., TN.
Pub. in Proceedings of Conference on Thermal Insulation, Materials, and System for Energy Conservation in the 80's, Clearwater Beach, FL., December 8-11, 1981, American Society for Testing and Materials Special Technical Publication 789, p248-264 1983.

Keywords: *Thermal insulation, *Thermal resistance, Heat flow meters, Tests, Calibrating, Energy conservation.

The design and procedure of a round-robin sponsored by ASTM C-16 using guarded hot-boxes (ASTM C-236) and calibrated hot-boxes (ASTM C-draft in process) is described. A description of an International Standards (ISO) sponsored round-robin of tests using guarded hot-plate and heat flow meter apparatuses to measure the thermal resistance of thick thermal insulation materials is given. A brief summary of a three phase round-robin program sponsored by the ASTM C-16.30 Subcommittee on Thermal Measurements and the Mineral Insulation Manufacturers Association (MIMA) on several types of glass fiber insulation material is given.

501,260

PB86-112885 Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Fields Div.

Orbiting Standards Package: A Recalibratable Satellite Instrument Assembly for Measuring Large Earth Station Antennas.

Final rept.,
A. J. Estin, and R. C. Baird. 1982, 12p
Pub. in Proceedings of the Antenna Measurements Symposium, Las Cruces, New Mexico, October 5-7, 1982, p5-1-5-12.

Keywords: *Antennas, Artificial satellites, Measuring instruments, Electromagnetic radiation, Microwave communication, *Orbiting Standards Package, Earth terminals, Electromagnetic measurement.

The concept of an Orbiting Standards Package (OSP) has been discussed as a means of making direct measurements of fields, patterns, and polarization states of signals radiated from large earth station antennas. It would also have the capability of producing test fields of known intensities and arbitrary but well-defined polarization states, thereby enabling the determination of such parameters as G/T and Effective Receiving Area of earth stations. Recent developments in microwave six-port networks and in standard antennas would permit the all-electronic generation and detection of these signals. Moreover, it appears possible to recalibrate the satellite standards package to laboratory state-of-the-art accuracy following launch.

501,261

PB86-112901 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Center for Analytical Chemistry.

Analytical Optogalvanic Spectroscopy in Flames.

Final rept.,
J. C. Travis. 1985, 1p
Pub. in Analytical Laser Spectroscopy, p213-233 1985.

Keywords: *Chemical analysis, *Ionization, Excitation, Design criteria, Performance evaluation, Reprints, *Laser spectroscopy, *Optogalvanic spectroscopy, *Laser enhanced ionization, Flame spectroscopy.

Optogalvanic spectroscopy is based on changes in the impedance of a weakly ionized plasma in response to the optical excitation of an atomic or molecular species in the plasma. Though rooted in research of over five decades ago, optogalvanic spectroscopy has flourished with the advent of tunable lasers. Optogalvanic spectroscopy in flames, or laser enhanced ionization, has been extensively developed as a flame spectrophotometric analytical method. This paper reviews the research into the theory and practice of laser enhanced ionization since the inception of the method in 1976. The mechanisms of ion production, ion transport, and signal generation are treated theoretically, and supported by experimental studies. The development of analytical LEI is presented, with discussions of instrumentation, sensitivity, and accuracy.

501,262

PB86-113628 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Building Physics Div.

Thermal Testing of Passive/Hybrid Solar Components.

Final rept.,
M. E. McCabe. 1982, 6p
Sponsored by Department of Energy, Washington, DC. Passive and Hybrid Solar Energy Div.
Pub. in Proceedings of Passive and Hybrid Solar Energy Update, Washington, DC., September 15-17, 1982, p251-256.

Keywords: *Test facilities, *Solar heating, Buildings, *Passive solar heating systems, Solar space heating.

Studies of thermal performance of passive solar buildings have indicated a need for precise field measurement of solar heat gain and thermal heat loss or gain for modular passive/hybrid solar components. A description of the conceptual design and the major assemblies and subsystems for a new calorimetric test facility is presented. The facility is designed for field testing of passive solar components at the National Bureau of Standards in Gaithersburg, MD. The test facility metering chamber can accommodate test articles having nominal dimensions up to 1.26 x 2.09 m corresponding to a standard sliding door, with thicknesses up to 0.41 m (16 in). The test articles are installed in the buildings envelope and can be oriented either to the vertical-south, or to the horizontal-upward facing direction. The metering chamber is designed to simulate an ideal indoor thermal environment by absorbing all the solar energy transmitted by the test article and by maintaining the indoor air and surface temperatures at controlled values between 15.6 and 26.7°C (60 and 80°F). A description of the passive/hybrid solar components proposed for testing in the calorimeter during the winter season of 1982-1983 is provided.

501,263

PB86-113669 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.

General Purpose Atom Probe Field Ion Microscope.

Final rept.,
A. J. Melmed, M. Martinka, and R. Klein. 1982, 6p
Pub. in Proceedings of International Field Emission Symposium (29th), Goteborg, Sweden, August 9-13, 1982, p243-248.

Keywords: Design criteria, Performance evaluation, Spectrochemical analysis, Mass spectroscopy, *Atom probe field ion microscopy.

A general purpose atom probe field ion microscope is described and the initial results are discussed. The UHV instrument combines the capabilities of a straight ToF Atom Probe and an Imaging Atom Probe, with a specimen-detector distance of 14 cm. Novel features are a variable aperture and a specimen quick-change

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Group 14B—Laboratories, Test Facilities, and Test Equipment

which allows preservation of input pulse line integrity. Mass resolution is about 200 at 15% peak height and appears to be independent of probe anular diameter between 15 and 65 deg.

501,264
PB86-115557 Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div.
Accurate Noise Measurements of Superconducting Quasiparticle Array Mixers.
Final rept.,
W. R. McGrath, A. V. Ræisaenen, P. L. Richards, R. E. Harris, and F. L. Lloyd. 1985, 4p
Sponsored by Office of Naval Research, Arlington, VA. Pub. in IEEE (Institute of Electrical and Electronics Engineers) Transactions on Magnetics MAG-21, n2 p212-215 Mar 85.

Keywords: *Mixing circuits, *Electromagnetic noise, *Josephson junctions, Microwave equipment, Superconductors, Measurement, Reprints, Microwave sensors.

The authors have constructed a 30-40 GHz test apparatus which allows us to measure the noise temperatures of SIS mixers with an accuracy of better than ± 1 K. This is a factor of six improvement over earlier measurements. In addition, SIS mixers employing arrays of $N = 1, 5, 10, 25$, and 50 tunnel junctions in series have been tested. The input power required to saturate the array mixers was found to increase as N squared, and the gain and noise temperature of the array mixers were independent of N .

501,265
PB86-119393 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.
Characterization of NBS (National Bureau of Standards) Standard Reference Material 2135 for Sputter Depth Profile Analysis.
Final rept.,
J. Fine, and B. Navinsek. 1985, 5p
Pub. in Jnl. of Vacuum Science and Technology A3, n3 p1408-1412 May/June 85.

Keywords: *Sputtering, Ion beams, Calibrating, Interfaces, Resolution, Thin films, Nickel, Chromium, Reprints, *Standard reference materials, Auger spectroscopy.

A Ni/Cr multilayered thin-film standard reference material (SRM) for sputter depth profile calibration has been developed jointly by the National Bureau of Standards, the Jozef Stefan Institute, and the American Society for Testing and Materials (ASTM) Committee E-42 on Surface Analysis. This periodically modulated structure can be effectively used to calibrate sputter erosion rates and depth of erosion scales in surface analysis as well as to monitor ion beam stability and to optimize sputtering conditions so as to achieve maximum interface resolution. Characterization results obtained on this first SRM for surface analysis to be issued by NBS indicate that the accuracy of its structure is known to better than 6% and that its sputter profiles are well defined and reproducible. Results of the calibration and compositional analysis of this SRM are presented regarding uniformity and periodicity of thin film layers, absolute film thickness, sputtered interface depth resolution, and relative Ni/Cr sputtering rates and yields. Measurement methods used to characterize this thin-film structure include EN(E) Auger sputter depth profiling, Rutherford backscattering spectrometry, and neutron activation analysis.

501,266
PB86-121597 PC A13/MF A01
National Bureau of Standards (NML), Gaithersburg, MD. Center for Basic Standards.
Technical Activities 1983, Center for Basic Standards.
Final rept.,
K. G. Kessler. Jan 84, 276p NBSIR-83/2793
See also PB85-164952.

Keywords: *Research, *Standards, Metrology, Fundamental constants, Pressure, Gravity, Lasers, Length, Mass, Vacuum, Time standards, Frequency standards, X rays, Gamma rays, Temperature, Electrical measurement, Laser applications.

The report is Part II of the 1983 Annual Report of the Center for Basic Standards and contains a summary of the technical activities of the Center for the period Oc-

tober 1, 1982 to September 30, 1983. The Center is one of the five resources and operating units in the National Measurement Laboratory.

501,267
PB86-122751 Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Fields Div.
E and H Fields in Transmission Lines and Coils for Susceptibility Testing, Probe Calibration, and RF Exposure Chambers.
Final rept.,
E. B. Larsen, and J. E. Cruz. 1985, 1p
Proceedings of IEEE (Institute of Electrical and Electronics Engineers) Instrumentation and Measurement Technology Conference (IMTC '85), Tampa, FL., March 20-22, 1985, p199.

Keywords: *Electromagnetic compatibility, Transmission lines, Electromagnetic fields, Measurement, Transverse waves, Calibrating, Electric coils, Test equipment, Tests, TEM cells.

The paper deals with the instrumentation and design equations for several systems used to generate calculable electric (E) and magnetic (H) fields for electromagnetic compatibility (EMC) testing. These 'standard' electromagnetic (EM) fields with known magnitude are used to: (a) test the susceptibility of electronic equipment to radiated fields, (b) calibrate E and H field probes for measuring and mapping fields, and (c) expose biological specimens in a known EM environment.

501,268
PB86-122777 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Electrosystems Div.
Approach to ATE (Automatic Test Equipment) Calibration via Performance Verification at the System Interface.
Final rept.,
T. F. Leedy. 1985, 4p
Pub. in Proceedings of 1985 Measurement Science Conference, Santa Clara, CA., January 17-18, 1985, p198-201.

Keywords: Performance evaluation, Calibrating, *Automatic test equipment.

A method of verifying the performance of automatic test equipment (ATE) in its normal operating environment and configuration is presented as the best approach to achieving an overall system calibration. The method consists of the transport of well-characterized signal sources to the ATE station and the application of these electrical stimuli directly to a well-defined electrical interface on the test station.

501,269
PB86-122793 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.
Experimental Program at the National Bureau of Standards Synchrotron Ultraviolet Radiation Facility (SURF).
Final rept.,
R. P. Madden, D. L. Ederer, and A. C. Parr. 1985, 4p
Sponsored by National Aeronautics and Space Administration, Washington, DC., and Office of Naval Research, Arlington, VA.
Pub. in Nuclear Instruments and Methods in Physics Research B10/11, p289-292 1985.

Keywords: Far ultraviolet radiation, Synchrotron radiation, Surface properties, Photodiodes, Calibrating, Reprints, *Surf II storage ring, Photoelectron spectroscopy.

New beamline development on SURF features toroidal grating instruments for Surface Science studies and Far UV photodiode calibration. The progress and capabilities of these lines will be discussed along with the developments on the high resolution normal incidence spectrometer beam line under construction by the University of Maryland. The ongoing programs in Surface Science and Photoelectron Spectroscopy are reviewed briefly, with a more detailed discussion of the latest results in calibration efforts using electron counting and the calculable spectral distribution of synchrotron radiation.

501,270
PB86-122819 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD.

Statistical Analysis of Sampling and Measurement Errors in the Characterization of Refuse Derived Fuel.

Final rept.,
J. Mandel, and R. C. Paule. 1981, 6p
Pub. in Proceedings of International Symposium on Materials and Energy from Refuse, Antwerp, Belgium, October 20, 1981, p6.25-6.30.

Keywords: *Statistical analysis, *Error analysis, *Calorific value, *Ash content, *Chemical analysis, Sampling, Graphs(Charts), Heat measurement, *Refuse derived fuels, *Municipal wastes, Numerical solution.

A statistical analysis is presented, giving results of a sampling experiment involving a production stream of Refuse Derived Fuel. Calorimetric and ash measurements were analyzed and statistical parameters were estimated. Measures were obtained for the variability of the material both within and between days of production, and for the errors of measurement. Particular attention was given to the relation between the ash and heat measurements. The results are presented in numerical and graphical form.

501,271
PB86-122884 Not available NTIS
National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.
Calibration Methods for Eddy Current Measurement Systems.
Final rept.,
J. C. Moulder, J. C. Gerlitz, B. A. Auld, M. Riazat, and S. Jeffries. 1985, 10p
Pub. in Proceedings of Review of Progress in Quantitative Nondestructive Evaluation, San Diego, CA., July 8-13, 1984, v4A p411-420 1985.

Keywords: *Eddy currents, Calibrating, Nondestructive tests, Measurement.

Quantitative inversion of eddy current signals to obtain flaw sizes from actual measurements requires methods for calibrating eddy current measurement systems. In performing flaw-signal inversion it is not sufficient to know the phase of the flaw signal relative to lift-off; rather, the absolute phase of Delta Z is required. The authors explore three possible approaches to this problem: absolute electrical calibration of the measurement system, measurements of probe lift-off signals, and measurements on actual or simulated flaws. Air core, circular coils of rectangular cross-section are used to facilitate comparisons of theory and observation. Results of lift-off measurements are found to agree with analytical solutions obtained by Dodd and Deeds. Flaw signals for rectangular-shaped, surface-breaking flaws agree with the predictions of the nonuniform-probe-field theory of Muennemann and Auld.

501,272
PB86-122918 Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Fields Div.
Noise Temperature Measurements at the National Bureau of Standards.
Final rept.,
S. Perera. 1985, 2p
Pub. in Proceedings of IEEE (Institute of Electrical and Electronics Engineers) Instrumentation and Measurement Technology Conference (IMTC '85), Tampa, FL., March 20-22, 1985, p159-160.

Keywords: *Thermal noise, *Radiometers, Measurement, Sources.

Thermal noise presents the ultimate limitation in the reception and detection of low level electromagnetic signals. This paper briefly reviews the physics of thermal noise, devices that generate noise, and measurement methods to characterize noise sources.

501,273
PB86-122934 Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Fields Div.
Standards for Measurement of Electromagnetic Fields.
Final rept.,
M. Kanda, and N. S. Nahman. 1985, 4p
Pub. in Proceedings of IEEE (Institute of Electrical and Electronics Engineers) Instrumentation and Measurement Technology Conference (IMTC '85), Tampa, FL., March 20-22, 1985, p20-23.

Keywords: *Electromagnetic fields, Measurement, An-echoic chambers, Standards.

The standards developed at NBS for measurements of electromagnetic fields will be reviewed along with the industrial applications that engendered their development. Some attention will be given to future measurement requirements and the NBS programs to meet them.

501,274
PB86-123015 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD.

Ultra-High Resolution Frequency Meter.

Final rept.,
J. J. Snyder. 1981, 6p
Pub. in Proceedings of Annual Frequency Control Symposium (35th), Philadelphia, PA., May 27-29, 1981, p464-469.

Keywords: *Frequency meters, Frequency measurement, Random noise, Signal to noise ratio.

The authors have recently developed a novel instrument for measuring the frequency of a periodic signal contaminated by random phase noise. This frequency meter averages overlapping time intervals using a simple algorithm implemented with standard logic circuits. Because of the signal-to-noise improvement inherent in the averaging process, the standard deviation of a single measurement contaminated by, e.g., white phase noise is proportional to τ to the minus 1.5 power, τ is the time for the measurement. In contrast, the uncertainty in the measurement of the frequency of a noisy signal using a standard frequency counter is proportional to $1/\tau$. For many potential applications of the frequency meter, the measurement uncertainty due to contaminating noise may thereby be reduced by several orders of magnitude in comparison with a measurement over the same time interval using presently available instruments.

501,275
PB86-123031 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Mechanical Production Metrology Div.
Evaluation of Methods for Characterizing Surface Topography of Models for High Reynolds Number Wind-Tunnels.

Final rept.,
E. C. Teague, T. V. Vorburger, F. E. Scire, S. W. Jensen, and S. M. Baker. 1982, 6p
Pub. in American Institute of Aeronautics and Astronautics Aerodynamic Testing Conference (12th), Williamsburg, VA., March 22-24, 1982, p246-251.

Keywords: *Wind tunnels, Evaluation, Wind tunnel models, Reynolds number, Boundary layer flow.

Because of the high Reynolds number of the National Transonic Facility, (NTF), and the attendant thin boundary layers, NASA is reexamining aerodynamic effects related to model surface topography definition. There are no data which demonstrate that the stylus profilometers used by model fabrication shops accurately determine the surface topography of surfaces typical of NBS models. The paper describes current work at the National Bureau of Standards, sponsored by NASA, to evaluate the performance of stylus profilometers for this application and to develop a light scattering instrument which will yield accurate characterizations of the surface microtopography and overcome the problems associated with stylus profilometry.

501,276
PB86-123080 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.

Quantitative Acoustic Emission Studies for Materials Processing.

Final rept.,
H. N. G. Wadley, C. K. Stockton, J. A. Simmons, M. Rosen, and S. D. Ridder. 1982, 11p
Pub. in Proceedings of Air Force/Defense Advanced Research Projects Agency Symposium (8th), Boulder, CO., August 2-7, 1981, Review of Progress in Quantitative Nondestructive Evaluation 1, p421-431 1982.

Keywords: Acoustics, Q switched lasers, Greens function, Wave propagation, Nondestructive tests, *Acoustic emission testing, *Rapid solidification.

The techniques being developed in Rapid Solidification Technology (RST) can be used to improve and

critically evaluate the performance of acoustic emission methods for nondestructive evaluation (NDE). In turn, these NDE techniques could play an important part in the development of advanced materials. The paper first describes the use of a Q-switched laser for the generation of predictable acoustic emission signals which are to be used to evaluate quantitative multichannel source characterization methods. Second, the laser generation of elastic waves is used to measure the speed of extensional wave propagation in metallic glass ribbons, and to thus deduce the degree of crystallization as a function of isothermal annealing.

501,277
PB86-124153 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD.

Preliminary Industrial Evaluation of the Fluidic Capillary Pyrometer.

Final rept.,
R. M. Phillippi, and T. Negas. 1980, 6p
Sponsored by Harry Diamond Labs., Adelphi, MD.
Pub. in Proceedings of Winter Annual Meeting of ASME (American Society of Mechanical Engineers) Anniv. Fluid Symposium, Chicago, IL., November 16-21, 1980, p31-36.

Keywords: Temperature measuring instruments, Evaluation, *Fluidic temperature sensors.

The paper presents results from a preliminary field evaluation of the fluidic capillary pyrometer (FCP). The device uses a viscosity and hence temperature-sensitive fluid resistor, or capillary tube as the sensing element in a simple fluid resistor bridge. Resultant pressure changes due to temperature (typically quite small for a gas) are then amplified to a useful level with fluidic laminar pressure amplifiers. Data are shown for over 2000 hours of operation, accumulated by two FCP units in a U.S. Army rotary hearth forging furnace (1200 C) with sensing probes of alumina operating on air.

501,278
PB86-124914 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Office of the Director.
How Good Are the Standard Atomic Weights.
Final rept.,
H. S. Peiser. 1985, 6p
Pub. in Analytical Chemistry 57, n511A 1985.

Keywords: *Chemical elements, *Standards, Isotopes, Samples, Reprints, *Natural emissions, *Atomic weights.

The tables of atomic weights of the chemical elements as they are found in natural terrestrial sources are reviewed regularly and published by the International Union of Pure and Applied Chemistry. After a recent major revision of these tables, the author discusses the improvement and limitations in the reliability of these data as they affect analytical chemists. The uncertainty of these data are implied in the precision of the tabulated numerical values. Taken into account are both experimental uncertainties and natural variability of isotopic abundances. The 20 elements that have only one stable nuclide have atomic weights reliable to about 1 part in 10,000,000. An equal number of elements have experimental uncertainties of more than 1.5 parts in .0001 with no significant variability. Their atomic-weight determination remains a challenge to experimenters. About 11 elements are so variable that atomic weights of given samples can be measured more accurately than the atomic weight values have been tabulated. Radioactive decay affects appreciably only the atomic weights of daughter elements in some abnormal sources.

501,279
PB86-124971 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Temperature and Pressure Div.

Thermometry in Coal Utilization.

Final rept.,
J. F. Schooley. 1982, 8p
Pub. in Proceedings of Symposium on Instrumentation and Control for Fossil Energy Processes, Houston, TX., June 7-9, 1982, p161-168.

Keywords: *Coal preparation, *Temperature measurement, Substitutes.

Thermometry techniques suitable for use in coal processing are discussed. Common problems encountered in the use of thermocouple thermometers are summa-

rized. Alternative methods, including velocity-of-sound, Johnson noise, and various blackbody and spectroscopic measurements are outlined. Some 27 references to literature on these topics are included.

501,280
PB86-128774 Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
Effect of Ion Current in the Collisionless Theory of Floating AC Probe Measurements. Final Report,
E. R. Mosburg. 1981, 5p
See also PB82-118357.
Pub. in Review of Scientific Instruments 52, n8 p1182-1186 Aug 81.

Keywords: *Langmuir probes, Electron energy, Plasma diagnostics, Reprints, *Electron temperature.

Previous treatment of the theory of floating ac probes has considered only the electron current voltage dependence. In the paper the effect of including the voltage dependence of the ion current is examined, and equations are derived which allow the use of the calculations by Laframboise of the ion current to cylindrical probes having arbitrary ratios of probe diameter to Debye length. The error in electron temperature measurements introduced by neglecting the ion current variation, and the range of usefulness of the technique, is discussed. For example, in the normally expected range of floating potential, a measurement of the electron temperature could be in error by as much as about 13% if the voltage dependence of ion current is ignored.

501,281
PB86-128824 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD.
Fluidic Capillary Temperature Sensors: Materials, Design and Fabrication.

Final rept.,
T. Negas, H. S. Parker, W. S. Brower, R. M. Phillippi, and T. M. Drzewiecki. 1980, 7p
Pub. in Proceedings of ASME (American Society of Mechanical Engineers) Symposium on Fluid (20th), Chicago, IL., November 16-21, 1980, p37-43.

Keywords: Temperature measuring instruments, Capillary flow, Refractory metal alloys, Molybdenum, Detectors, Design, Fabrication, *Fluidic temperature sensors.

Prototype fluidic capillary pyrometers (FCP) were designed and fabricated to measure temperature well above 1200 degrees C. Monolithic ceramic sensors were constructed from several refractory oxides to demonstrate that processing is feasible and to evaluate performance of the FCP at elevated temperature. Sensors, constructed from refractory metals such as molybdenum, are attractive for applications where rapid response and resistance to high thermal stress are important factors.

501,282
PB86-128857 Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Time and Frequency Div.
Accuracy of International Time and Frequency Comparisons via Global Positioning System Satellites in Common-View.

Final rept.,
D. W. Allan, D. D. Davis, M. Weiss, A. Clements, and B. Guinot. 1985, 8p
Pub. in IEEE (Institute of Electrical and Electronics Engineers) Transactions on Instrumentation and Measurement IM-34, n2 p118-125 Jun 85.

Keywords: *Frequency standards, *Time standards, *Accuracy, Measurement, Reprints, Global positioning system.

Frequency differences between major national timing centers are being resolved with uncertainty of less than 1 part in 10 to the 14th power, using satellites of the Global Positioning System (GPS) in common-view. Portable clock and GPS time differences are in excellent agreement. Around the world GPS measurement between three laboratories had a time residual of 5.1 ns.

501,283
PB86-128923 Not available NTIS

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Group 14B—Laboratories, Test Facilities, and Test Equipment

National Bureau of Standards (NML), Boulder, CO.
Time and Frequency Div.

Frequency and Time Coordination, Comparison, and Dissemination.

Final rept.,
D. W. Allan. 1985, 41p
Pub. in Precision Frequency Control 2, p233-273 1985.

Keywords: *Time standards, *Frequency standards, *Calibrating, Metrology, Coordination, Comparison, Reprints.

The purpose of the chapter is to review both the current and some anticipated metrology techniques useful in comparing or calibrating remotely located time and frequency standards. Typically, the interest in this regard is to make available to a remote user some primary frequency or time standard reference. The techniques usually employed to accomplish this either involve the transport of a secondary standard or the propagation of time and frequency information carried on an electromagnetic signal. The accuracy, reasonable coverage areas, convenience to the user, and, in some cases, nominal cost of some of these techniques of comparison and dissemination will be reviewed.

501,284
PB86-128964 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Gas and Particulate Science Div.

Raman Microprobe Spectroscopic Analysis.

Final rept.,
J. J. Blaha. 1981, 41p
Pub. in Vibrational Spectra and Structure: A Series of Advances, v10 p227-267 1981.

Keywords: *Raman spectroscopy, *Microanalysis, *Molecular vibration, Particles, Sampling, Laboratory equipment, Forecasting, Molecular structure, Chemical analysis, Reprints.

Raman microprobe and microscopes have extended vibrational spectroscopy to the analysis of microparticles whose dimensions are on the order of micrometers. These techniques have been applied to the analysis of a wide variety of materials in a broad range of fields. Many of these investigations have been demonstrations of potential while others have yielded information that can not be obtained by any other technique. Raman spectra obtained from microparticles are directly related to that from both samples. In contrast to the measurement of macroscopic crystals, all of the Raman active modes of a sample are usually observed in a single spectrum when microparticles are examined. In this review, a general summary of the Raman microprobe technique, instrumentation and applications will be made to demonstrate the versatility of the technique to a wide range of problems. In addition some information is presented on possible future developments in applications and improvements in instrumentation.

501,285
PB86-128998 Not available NTIS
National Bureau of Standards (NML), Boulder, CO.
Time and Frequency Div.

Frequency and Time Standards Based on Stored Ions.

Final rept.,
J. J. Bollinger, D. J. Wineland, W. M. Itano, J. C. Bergquist, and J. D. Prestage. 1985, 10p
Sponsored by Air Force Office of Scientific Research, Bolling AFB, DC., and Office of Naval Research, Arlington, VA.
Pub. in Proceedings of Annual Precise Time and Time Interval Applications and Planning Meeting (16th), Greenbelt, MD., p49-58 1985.

Keywords: *Time standards, *Frequency standards, Atomic clocks, Microwaves, Doppler effect, *Ion storage, Ion traps, Penning traps, Laser cooling.

The method of ion storage provides a basis for excellent time and frequency standards. This is due to the ability to confine ions for long periods of time without the usual perturbations associated with confinement (e.g. wall shifts). In addition Doppler effects can be greatly suppressed. The use of stored ions for microwave frequency standards and the future possibilities for an optical frequency standard based on stored ions are addressed.

501,286
PB86-129020 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.

Reference Materials: Their Production, Certification and Use in Compatible Measurement Networks.

Final rept.,
J. P. Cali. 1979, 20p
Pub. in Proceedings of Euroanalysis III, Reviews in Analytical Chemistry, p153-172 1979.

Keywords: *Measurements, *Chemical analysis, Laboratory equipment, *Reference materials, Certified reference materials, Standard reference materials.

In a world becoming increasingly interdependent in terms of trade, environmental protection, safeguarding of nuclear materials, and world health, among others, the importance of being able to make dependable and reliable measurements is self-evident. Measurement compatible networks are designed and their work implemented in a manner that assures that measurement results from one laboratory to another agree within predetermined uncertainties useful for some stated end-purpose. Networks that accomplish accurate measurements, (measurements free of systematic error and precise), produce results that are compatible. One important mode for achieving accurate measurements, especially useful for the determination of chemical composition, is based on the use of reference materials in the measurement process. The production and certification of reference materials (RM's) is a complex, time-consuming, and costly process requiring measurement resources of the highest order in terms of skilled manpower and sophisticated equipment. To describe and illustrate these, the author uses as his model the RM program of the U.S. National Bureau of Standards, a program now approaching its 80th anniversary. Of great importance, is the scientific integrity and credibility of the finished product. The three measurement modes used at NBS to arrive at certifiable values for its RM's are described in some detail. General principles involved in RM production are also discussed.

501,287
PB86-129038 Not available NTIS
National Bureau of Standards (NEL), Boulder, CO.
Electromagnetic Technology Div.

Precision Measurement of Eddy Current Coil Parameters.

Final rept.,
T. E. Capobianco, and F. R. Fickett. 1985, 8p
Pub. in Review of Progress in Quantitative Nondestructive Evaluation 4A, p491-498 1985.

Keywords: *Coils, *Eddy current tests, Precision, Impedance, Phase angle, Inductance, Deformation, Oscilloscope, Reprints.

Precision measurements of impedance, phase angle, and dissipation factor of both commercial eddy current coils and specially prepared test coils by various techniques are described. Special emphasis is placed on use of the digital storage oscilloscope and commercial LCZ meter. Detection of the effect on the coil parameters of shorted turns, deformation, and ferrite defects is described.

501,288
PB86-129541 PC A04/MF A01
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Chemical Engineering.
Review of Materials for pH Sensing for Nuclear Waste Containment,
T. Dietz, and K. G. Kreider. Sep 85, 62p NBSIR/85-3237
Sponsored by Nuclear Regulatory Commission, Washington, DC.

Keywords: *pH meters, *Radioactive wastes, Reviews, Corrosion, Design criteria, Performance evaluation, Electrochemistry, Electrodes, Glass, Thin films, Platinum oxides, Stability, Transition metals, Yttrium compounds, *Radioactive waste disposal, *Radioactive waste storage, NRC, Chemical reaction mechanisms, Metal oxides, Palladium hydride, Iridium oxide.

The report defines the performance criteria of the needed pH sensors and reviews the performance of a number of elevated temperature pH sensing technologies with respect to these criteria. The criteria of electrode performance were developed to predict the utility of various pH electrodes in these simulated environments. The classes of pH electrodes reviewed are the glass electrode, yttria stabilized zirconia, palladium hydride and a variety of metal oxides. The report focuses on a relatively new solid state electrode material, reactively sputter deposited iridium oxide. The perform-

ance of this thin film material is of particular interest because its low electrical resistivity and high corrosion resistance eliminate some of the shortcomings of the glass and ceramic materials. The reactive sputtering technology permits these films to be deposited and pattern defined on a wide variety of substrate materials. Low electrical resistivity, which simplifies electrical contacts, and a flexible deposition technology make this material a prime candidate for micro pH sensors.

501,289
PB86-129616 Not available NTIS
National Bureau of Standards (NEL), Boulder, CO.
Electromagnetic Technology Div.

Superconductor-Insulator-Superconductor Quasiparticle Junctions as Microwave Photon Detectors.

Final rept.,
P. L. Richards, T. M. Shen, R. E. Harris, and F. L. Lloyd. 1980, 3p
Sponsored by Office of Naval Research, Arlington, VA.
Pub. in Applied Physics Letters 36, n6 p480-482, 15 Mar 80.

Keywords: Microwave equipment, Electron tunneling, Superconductors, Detectors, Reprints, *Microwave sensors, Quasiparticles.

The strong nonlinearity of the quasiparticle tunneling current in superconductor-insulator-superconductor junctions near the full-gap voltage $2\Delta/e$ can be used for direct detection of microwave signals. Measurements at 36 GHz yielded a current responsivity of 3500 A/W, which is within a factor of 2 of the quantum-limited value $e/(h\bar{\omega})$. The measured NEP of $2.6 \pm 0.8 \times 10^{-16}$ W/(Hz sup 1/2) is the lowest value reported to date and can probably be improved significantly. The experimental results are compared with both the standard classical analysis and photon-assisted tunneling theory.

501,290
PB86-129624 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Statistical Engineering Div.

Nonparametric Calibration.

Final rept.,
G. Knafl, J. Sacks, C. Spiegelman, and D. Ylvisaker. 1984, 9p
Pub. in Technometrics 26, n3 p233-241 Aug 84.

Keywords: *Calibrating, Mathematical models, Reprints, Systematic errors.

The paper deals with calibration when a linear model may not hold exactly. Usually, a calibration curve f is assumed to follow a linear model, e.g., $f(x) = a + bx$ or $f(x) = a + bx + c(x \text{ squared})$. As such calibration curves only approximate reality, there is a discrepancy between the assumed linear model and the true curve. This discrepancy produces systematic errors in the measurements obtained from the fitted calibration curve. The new procedures recommended here cope directly with such systematic errors, whereas the more traditional linear model approach cannot.

501,291
PB86-129756 PC A02/MF A01
National Bureau of Standards (NML), Gaithersburg, MD. Center for Radiation Research.

Radiometric Calibration Procedures Using the NBS (National Bureau of Standards) MARBLE Electronics Package.

Final rept.,
M. E. Mickelson, L. E. Larson, and J. Fowler. Sep 85, 23p NBS/TN-1216
Also available from Supt. of Docs as SN003-003-02692-1. Prepared in cooperation with Denison Univ., Granville, OH.

Keywords: *Radiometry, *Calibrating, Photodiodes, Marble.

The NBS MARBLE Electronics Package, which is designed to support calibration of radiometric detectors, including self-calibration of Si photodiodes, is described.

501,292
PB86-130234 PC A04/MF A01
National Bureau of Standards (NEL), Boulder, CO.
Electromagnetic Technology Div.

Laboratories, Test Facilities, and Test Equipment—Group 14B

Metrology for Electromagnetic Technology: A Bibliography of NBS (National Bureau of Standards) Publications.

K. E. Kline, and M. E. DeWeese. Jul 85, 70p NBSIR-85/3029
Supersedes PB85-112985, and PB83-111658.

Keywords: *Metrology, *Bibliographies, Fiber optics, Electromagnetic radiation, Superconductors, Lasers, Cryogenics, Josephson junctions, Microwaves, Waveforms, Time domain, National Bureau of Standards, SQUID devices.

The bibliography lists the publications of the personnel of the Electromagnetic Technology Division of NBS in the period from January 1970 through December 1984. A few earlier references that are directly related to the present work of the Division are included.

501,293
PB86-130358 PC A13/MF A01

National Bureau of Standards, Gaithersburg, MD.
Specifications, Tolerances, and Other Technical Requirements for Weighing and Measuring Devices as Adopted by the 70th National Conference on Weights and Measures, 1985 (1986 Edition).

Final rept.,
O. K. Warnlof. Sep 85, 293p NBS/HB-44
Supersedes PB85-157550. Also available from Supt. of Docs as SN003-003-02679-4.

Keywords: *Weight indicators, *Measuring instruments, *Handbooks, Specifications, Tolerances(Mechanics), Requirements, Standards.

Handbook 44 was first published in 1949, having been preceded by similar handbooks of various designations and in several forms beginning in 1918. This 1986 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 Bureau of Standards. It includes amendments adopted by the 70th Annual Meeting of the National Conference on Weights and Measures in 1985 and also a new Scales Code that will become effective January 1, 1986. Handbook 44 is published in its entirety each year following the Annual Meeting of the National Conference on Weights and Measures.

501,294
PB86-132602 Not available NTIS

National Bureau of Standards, Gaithersburg, MD.
Office of Nondestructive Evaluation.
Laser Generated and Detected Ultrasound and Holographic Methods.

Final rept.,
G. Birnbaum, G. S. White, and C. M. Vest. 1985, 9p
Sponsored by American Society of Mechanical Engineers, New York.
Pub. in Pressure Vessel and Piping Technology 1985: A Decade of Progress, p661-669 1985.

Keywords: *Holography, *Ultrasonic tests, Nondestructive tests, Ultrasonic radiation, Inspection, Pressure vessels, Laser radiation.

Several methods using laser radiation for nondestructive evaluation (NDE) are discussed. These include the noncontact generation of ultrasonic waves by the interaction of laser radiation with metal surfaces, and the noncontact detection of surface deformation due to ultrasonic waves by laser interferometric and knife-edge techniques. In addition, optical holography, which has been used for the inspection of pressure vessels, is discussed. Several applications for laser generation of ultrasonic waves are described.

501,295
PB86-132628 Not available NTIS

National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.
Wear Testing and Standardization.

Final rept.,
P. J. Blau. 1985, 3p
Pub. in ASTM (American Society for Testing and Materials) Standardization News, p34-36 Oct 85.

Keywords: *Wear tests, Standardization, Wear, Friction.

Wear exacts a high cost in our economy. Its many forms affect most technological disciplines. To improve control and reduction of wear, research and development programs need to use wear testing methods of many kinds. Standardization to only a few basic

tests may not be possible due to the diversity of wear modes. Use of simple, linear wear constants from laboratory tests may lead to unrealistic representations of actual component behavior. More advanced, multi-mode wear tests and analytical models for wear mechanisms need to be developed to improve relating laboratory testing data to field performance. ASTM can serve an important role by promoting multimode wear testing procedure development, improvements in standard terminology, and methods for reporting data.

501,296
PB86-132644 Not available NTIS

National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.
Microindentation Hardness Testing.

Final rept.,
P. J. Blau, and T. R. Shives. 1985, 5p
Pub. in ASTM (American Society for Testing and Materials) Standardization News 13, n1 p47-51 Jan 85.

Keywords: *Hardness tests, Metals, Microhardness, Microstructure, Failure.

The paper briefly reviews two common micro-indentation hardness testing methods for metals, highlighting sources of measurement errors, the need to understand the significance of microhardness numbers, and both traditional and more unique applications of such testing. Examples of studies from several applied fields are used to illustrate the points in the discussion: failure analysis, microstructural characterization, fracture mechanism research, and tribology. The trend towards automating hardness test methods is discussed.

501,297
PB86-133360 Not available NTIS

National Bureau of Standards (NEL), Boulder, CO.
Chemical Engineering Science Div.
Simple Gas Sampling and Injection Apparatus.

Final rept.,
T. J. Bruno. 1985, 3p
Sponsored by Gas Research Inst., Chicago, IL.
Pub. in Jnl. of Chromatographic Science 23, p325-327 Jul 85.

Keywords: *Gas chromatography, *Samplers, Injection, Laboratory equipment, Design criteria, Performance evaluation, Reprints.

The short paper describes a simple apparatus used for gas sampling and injection in gas chromatographic analysis. It can be constructed easily from commercially available equipment, and provides results which rival those obtainable from less conventional sampling systems. The main features of the sampler/injector are a variable volume sample reservoir and a standard tenport sampling valve equipped with an evacuable sample loop of fixed volume. The variable volume of the sample reservoir allows control of the sample pressure inside the loop. Evacuation of the sample loop prior to filling has been found to give a considerable increase in precision of replicate area count measurements. The sampler/injector is especially useful for situations in which a very limited amount of gaseous sample is available for analysis.

501,298
PB86-133386 Not available NTIS

National Bureau of Standards (NML), Gaithersburg, MD. Gas and Particulate Science Div.
Passive Sampler for Ambient Levels of Nitrogen Dioxide.

Final rept.,
B. C. Cadoff, and J. Hodgeson. 1983, 3p
Pub. in Analytical Chemistry 55, n13 p2083-2085 1983.

Keywords: *Nitrogen dioxide, *Monitors, *Air pollution, Sampling, Concentration(Composition), Laboratory equipment, Chemical analysis, Reprints, *Air pollution sampling, *Air pollution detection, *Passive monitors.

A precise, high-rate passive sampler for NO₂ is described. It can be assembled from a commercially-available device, and can be used to reliably sample low ambient levels of NO₂. Triethanolamine is used to collect the NO₂, and the analysis method follows the traditional Saltzman procedure. The device is diffusion controlled and samples at a rate of approximately 110 mL/min. It has been evaluated at two levels of relative humidity and exhibits no interference in the presence of a large excess of NO. Sampling has been conducted at 2 concentrations between 61 and 335 ppb.

501,299
PB86-133600 Not available NTIS

National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.

High-Resolution VUV Spectrometer with Multichannel Detector for Absorption Studies of Transient Species.

Final rept.,
C. L. Cromer, J. M. Bridges, J. R. Roberts, and T. B. Lucatorto. 1985, 16p
Sponsored by Air Force Office of Scientific Research, Bolling AFB, DC.
Pub. in Applied Optics 24, n18 p2996-3001, 15 Sep 85.

Keywords: *Ultraviolet spectrometers, Far ultraviolet radiation, Resolution, Image intensifiers, Reprints.

A new high-resolution VUV spectrometer is demonstrated for applications in the 40-900-A wavelength range. The instrument is comprised of a laser-plasma VUV source, which provides continuum background illumination, 1.5-m grazing incidence spectrometer, and a 1024-channel VUV optical multichannel analyzer (VUV-OMA). The VUV-OMA is of new design, featuring a special resolution enhanced channel electron multiplier array in an overall configuration chosen to optimize the spatial resolution of the detector while maintaining single-photoelectron sensitivity.

501,300
PB86-133626 Not available NTIS

National Bureau of Standards (NML), Gaithersburg, MD. Gas and Particulate Science Div.
Interlaboratory Comparison of Source Apportionment Procedures - Results for Simulated Data Sets.

Final rept.,
L. A. Currie, R. W. Gerlach, C. W. Lewis, W. D. Balfour, and J. A. Cooper. 1984, 21p
Pub. in Atmospheric Environment 18, n8 p1517-1537 1984.

Keywords: *Air pollution, *Aerosols, *Particles, Assessments, Sampling, Meteorology, Least square methods, Comparison, Sources, Reprints, State of the art, Intercomparison, Procedures.

Three sets of simulated compositional data for aerosol samples were prepared in order to (a) assess the current state of the art of source apportionment procedures, and (b) to provide initial sets of test data to aid in method development. The data sets were generated from reported source profile information, together with real meteorological data (St. Louis, 1976) and two constructed city plans. Following plume dispersion by means of the RAM model, forty 'samples' were generated having known source contributions and error structure. Deconvolution of the simulated data sets was undertaken by seven laboratories using numerical methods based primarily on least squares (Chemical Mass Balance) and multivariate (Factor Analysis and Multiple Linear Regression) techniques. Comparison of the interlaboratory results and estimated uncertainties with the known source contributions indicated consistency within about a factor of two (average about + or - 30%), and uncertainty estimates which ranged from much too conservative (broad) to much too small. No unique choice of method evolved from this exercise; the alternative methods appeared complementary and capable of resolving up to about 6-9 different sources. As a result of the intercomparison, suggestions are given for improving the simulation process per se, as well as the various methods of treating the data--especially with respect to the issue of estimated uncertainties.

501,301
PB86-133634 Not available NTIS

National Bureau of Standards, Gaithersburg, MD.
Many Dimensions of Detection in Chemical Analysis.

Final rept.,
L. A. Currie. 1983, 1p
Pub. in Abstracts of Papers of the American Chemical Society 185, p63 Mar 83.

Keywords: *Chemical analysis, Chromatographic analysis, Spectrochemical analysis, Mathematical models, Error analysis, Sampling, Calibrating, Reprints.

Simple detection decisions generally involve the comparison of scalar quantities (gross signal, blank). Conventional chromatography and spectrometry, on the other hand, involve one-dimensional variables (time, mass, wavelength, energy) where signal and baseline traces may be examined to decide whether a peak is present at a given location. Linked techniques, such as

Field 14—METHODS AND EQUIPMENT

Group 14B—Laboratories, Test Facilities, and Test Equipment

GC-MS or two-parameter nuclear spectroscopy, raise the question of detection in two dimensions. Finally, problems wherein a set of samples is characterized by many independent chemical and physical observations raise the issue of multidimensional detection. All such problems have a common theoretical base in the statistical theory of hypothesis testing. Following a brief review of underlying assumptions and techniques for applying the theory to detection decisions and detection limits, primary attention is given to a one-dimensional (reduced from two) problem involving the calibration curve of the pesticide Fenvalerate. Other topics addressed include information-loss through faulty reporting (at trace levels) and its impact on regulatory issues, and chemometric quality assurance through standard interlaboratory test data sets.

501,302
PB86-133642 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Temperature and Pressure Measurements and Standards Div.
Progress in Temperature Measurement.
Final rept.,
R. D. Cutkosky, R. E. Edsinger, J. P. Evans, and R. J. Soulen. 1983, 4p
Pub. in Proceedings of the ISA (Instrument Society of America) '83 International Conference and Exhibit, Landmarks in Metrology, Houston, TX., October 10-13, 1983, p13-16.

Keywords: *Temperature measurement, *Standards, Resistance thermometers, Resistance bridges, Thermocouples, Gas thermometers.

The authors review three articles which have had lasting impact on the measurement of temperature and the development of a temperature scale. The authors indicate the role they play in contemporary temperature standards.

501,303
PB86-136819 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Gas and Particulate Science Div.
Neutron Depth Profiling at the National Bureau of Standards.
Final rept.,
R. G. Downing, R. F. Fleming, J. K. Langland, and D. H. Vincent. 1983, 5p
Pub. in Nuclear Instruments and Methods in Physics Research 218, n1-3 p47-51, 15 Dec 83.

Keywords: *Neutrons, Nuclear reactions, Silicon, Helium 3, *Depth dose distributions, Semiconductors, Lithium 6, Boron 10, Sodium 22.

The National Bureau of Standards has established a dedicated neutron depth profiling (NDP) facility at its 10 MW research reactor in Gaithersburg, MD. The goal of the program is to provide real-time concentration profiles with the quality necessary to address scientific and technological problems. The depth profiles are obtained by deconvolution of energy spectra measured as monoenergetic charged particles are released by exoergic neutron reactions. The energy the particle retains upon leaving the sample surface is primarily dependent on the depth at which the reaction took place. Initially He-3, Li-6, B-10, and Na-22 are being studied because of their large thermal neutron cross sections and the importance of the nondestructive analysis of these elements in many matrices.

501,304
PB86-136850 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
High Frequency Optical Heterodyne Spectroscopy.
Final rept.,
M. Ducloy, and J. J. Snyder. 1983, 4p
Pub. in Proceedings of the Society of Photo-Optical Instrumentation Engineers Laser-Based Ultrasensitive Spectroscopy and Detection, San Diego, CA., August 23-24, 1983, v426, p87-90.

Keywords: *Doppler effect, *Noise reduction, Performance evaluation, *Laser spectroscopy, *Optical heterodyne spectroscopy.

The progress over the last few years in the field of sub-Doppler saturated absorption spectroscopy has been greatly assisted by the development of new techniques for increasing sensitivity. For many laboratory situations it is now routinely possible to achieve signal-to-noise ratios and sensitivities very near the quantum limit imposed by the fundamental statistical fluctua-

tions (shot noise) of the probe laser beam. It has been known for some time that the sensitivity of shot-noise limited saturation spectroscopy is exceedingly high. Until recently however, the sensitivity achieved in practice was more often several orders of magnitude worse than the predicted shot-noise limit. The reason for the reduced sensitivity is due to a number of non-fundamental or 'technical' sources, including common problems such as electronic interference and ground loops as well as amplifier noise, unstable laser feedback interference, and excessive laser amplitude noise. In this discussion the authors shall assume that the electronic problems have been solved, and that high-quality, low-noise amplifiers are in use. Their objective will be to show how the effects of laser feedback and laser amplitude noise may be reduced to the level of shot noise or below.

501,305
PB86-137635 (Order as PB86-137627, PC A04/MF A01)
National Bureau of Standards, Gaithersburg, MD.
Recalibration of the U.S. National Prototype Kilogram.
R. S. Davis. 14 Jun 85, 19p
Included in Jnl. of Research of the National Bureau of Standards, v90 n4 p263-283 Jul-Aug 85.

Keywords: *Mass, *Standards, *Units of measurement, *International prototype kilogram, *Kilogram.

The U.S. national prototype kilogram, K20, and its check standard, K4, were recalibrated at the Bureau International des Poids et Mesures (BIPM). Both these kilograms are made of platinum-iridium alloy. Two additional kilograms, made of different alloys of stainless steel, were also included in the calibrations. The mass of K20 in 1889 was certified as being 1 kg-0.039 mg. Prior to the work reported below, K20 was most recently recalibrated at the BIPM in 1948 and certified as having a mass of 1 kg-0.019 mg. K4 had never been recalibrated. Its initial certification in 1889 stated its mass as 1 kg-0.075 mg. The work reported below establishes the new mass value of K20 as 1 kg-0.022 mg and that of K4 as 1 kg-0.106 mg. The new results are discussed in detail and an attempt is made to assess the long-term stability of the standards involved with a view toward assigning a realistic uncertainty to the measurement.

501,306
PB86-137643 (Order as PB86-137627, PC A04/MF A01)
National Bureau of Standards, Gaithersburg, MD.
Density Comparison of Silicon Artifacts between NML (National Measurement Laboratory) (Australia) and NBS (National Bureau of Standards) (U.S.).
J. B. Patterson, and R. S. Davis. 6 Jun 85, 3p
Prepared in cooperation with National Measurement Lab., Chippendale (Australia).
Included in Jnl. of Research of the National Bureau of Standards, v90 n4 p285-287 Jul-Aug 85.

Keywords: *Silicon, *Density(Mass/volume), *Units of measurements, *Volume, Comparison, Standards, *Standard reference materials, *Artifacts.

The densities of four silicon artifacts were measured in SI units to .000001 by NML (Australia) and NBS (U.S.). Agreement is within the experimental uncertainty of each laboratory. Two of the artifacts had been used in the determination of the Avogadro constant at NBS. The remaining two objects had been used at NBS to establish silicon density artifacts available as a Standard Reference Material (SRM).

501,307
PB86-137650 (Order as PB86-137627, PC A04/MF A01)
National Bureau of Standards, Gaithersburg, MD.
Mass Comparator for In-Situ Calibration of Large Mass Standards.
R. M. Schoonover. 17 Jul 85, 6p
Included in Jnl. of Research of the National Bureau of Standards, v90 n4 p289-294 Jul-Aug 85.

Keywords: *Mass, *Standards, *Calibrating, *Units of measurement, *Mass comparators.

The paper describes a high precision electronic mass comparator with a range from 250 kg to 5,000 kg. It is suggested that it would be useful to transport the comparator to the test weights rather than to transport the weights to the comparator, the usual method, thus economizing time and monies.

501,308
PB86-137668 (Order as PB86-137627, PC A04/MF A01)
National Bureau of Standards, Gaithersburg, MD.
Determination of the Enthalpies of Combustion and Formation of Substituted Triazines in an Adiabatic Rotating Bomb Calorimeter.
W. H. Johnson, and E. J. Prosen. 28 Mar 85, 9p
Included in Jnl. of Research of the National Bureau of Standards, v90 n4 p295-303 Jul-Aug 85.

Keywords: *Enthalpy, *Combustion, *Triazines, *Calorimeters, Thermodynamic properties, Sampling, Thermochemistry, Laboratory equipment.

To obtain reliable thermodynamic data on substituted triazines, it is necessary to use a calorimeter that is capable of high precision with small quantities of sample and in which a homogenous solution of the corrosive combustion products can be maintained. The enthalpies of combustion of six substituted triazines have been determined in a platinum-lined adiabatic rotating bomb calorimeter. These are the first determinations of enthalpies of combustion or formation to have been reported for these compounds.

501,309
PB86-138039 Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div.
Magnetic Field Mapping with a SQUID (Superconducting Quantum Interference Device) Device.
Final rept.,
F. R. Fickett, and T. E. Capobianco. 1985, 10p
Pub. in Review of Progress in Quantitative Nondestructive Evaluation, v4A p401-410 1985.

Keywords: *Magnetic fields, *Magnetic measurement, Nondestructive tests, Eddy currents, Reprints, *SQUID (Detectors), SQUID devices.

Results of tests applying a SQUID (superconducting quantum interference device) system to measurement of the magnetic near field of commercial eddy current coils is reported. The SQUID system offers some significant advantages over more conventional techniques in that very small coils can be used and the calibration of the system is tied to the quantum of flux.

501,310
PB86-138070 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Gas and Particulate Science Div.
Review of Personal/Portable Monitors and Samplers for Airborne Particles.
Final rept.,
R. A. Fletcher. 1984, 3p
Pub. in Jnl. of the Air Pollution Control Association 34, n10 p1014-1016 Oct 84.

Keywords: *Monitors, *Air pollution, *Samplers, *Particles, Reviews, Design criteria, Performance evaluation, Reprints.

The operating characteristics of nineteen personal/portable particulate monitors are reviewed.

501,311
PB86-138179 Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Fields Div.
Picosecond Pulse Measurements at NBS (National Bureau of Standards).
Final rept.,
W. L. Gans. 1985, 3p
Pub. in Proceedings of IMTC '85 IEEE Instrumentation and Measurement Technology Conference, Tampa, FL., March 20-22, 1985, p142-144.

Keywords: *Electrical measurement, Minicomputers, Errors, *Picosecond pulses, Computer applications, Deconvolution.

The primary system used at NBS, Boulder, to measure fast (picosecond-nanosecond), repetitive, electrical pulse parameters consists essentially of a wideband (dc-18GHz) sampling oscilloscope interfaced to a minicomputer. The paper describes the techniques employed at NBS to reduce the effects of two major sources of pulse measurement error. These two sources are the distortions caused by the sampling head circuitry and by sample timing jitter. The techniques employed are based on the deconvolution methods of Tikhonov.

501,312
PB86-138351 Not available NTIS
 National Bureau of Standards (NEL), Gaithersburg, MD. Building Physics Div.
Acceptance Testing of the NBS (National Bureau of Standards) Calibrated Hot Box.
 Interim rept.,
 R. R. Jones. 1983, 16p
 Sponsored by Department of Energy, Washington, DC. Assistant Secretary for Conservation and Renewable Energy. Prepared in cooperation with American Society of Heating, Refrigerating and Air-Conditioning Engineers, Inc., Atlanta, GA.
 Pub. in ASHRAE/DOE Conference - Thermal Performance of the Exterior Envelopes of Buildings 2, Las Vegas, NV., December 6-9, 1982, p687-702 1983.

Keywords: *Calibrating, Testing, Walls.

The paper describes the acceptance testing requirements for a new calibrated-hot-box facility at the National Bureau of Standards, designed to permit simultaneous measurement of heat, moisture, and air flow in wall constructions while subjected to dynamic ambient conditions. The performance requirements specified for the calibrated hot box wall tester and the performance tests required to be met before final acceptance are discussed. Precision and accuracy considerations are set forth. The paper also proposes potential avenues of research and the issues related to carrying out a comprehensive testing program for evaluation of the performance of wall sections.

501,313
PB86-138542 Not available NTIS
 National Bureau of Standards (NEL), Boulder, CO. Thermophysical Properties Div.
Status of Thermal Conductivity Standard Reference Materials at the National Bureau of Standards.
 Final rept.,
 J. G. Hust. 1985, 12p
 Pub. in Therm. Conduct. 18, p327-338 1985.

Keywords: *Thermal conductivity, *Standards, Metals, Tungsten, Iron, Stainless steel, Graphite, Calibrating, Reprints, *Standard reference materials.

The paper describes the present status of NBS thermal conductivity Standard Reference Materials (SRM's) and Calibrated Transfer Specimens (CTS's). Included are the metal SRM's, tungsten, electrolytic iron, and austenitic stainless steel. Also discussed is graphite, a soon-to-be-established SRM and candidate SRM's, such as black quartz. Finally, a description is given of the insulation SRM's and CTS's.

501,314
PB86-139821 Not available NTIS
 National Bureau of Standards, Gaithersburg, MD.
Laboratory Evaluation Process of the National Voluntary Laboratory Accreditation Program.
 Final rept.,
 M. V. Federline. 1983, 9p
 Proceedings of Symposium on Evaluation and Accreditation of Inspection and Test Activities, ASTM STP 814, p96-104 1983.

Keywords: *Test facilities, *Quality assurance, Laboratories, *Accreditation, National Voluntary Laboratory Accreditation Program, NVLAP program.

At least 70 laboratory accreditation systems exist in the United States today, many of which are directed at a single discipline or narrow spectrum of products. The increase in the number of these systems in response to a growing need for laboratory testing services indicates the viability of the laboratory accreditation concept. The National Voluntary Laboratory Accreditation Program (NVLAP) was established by the Department of Commerce to provide a national, multidisciplinary laboratory evaluation scheme. NVLAP evaluation is based upon compliance with criteria which reflect the latest technology in laboratory operation and management. These criteria are sufficiently flexible to accommodate such diverse testing areas as thermal insulation, carpet, and concrete. The evaluation of laboratories, conducted by the National Bureau of Standards uses a peer review. It combines elements of questionnaire, laboratory on-site survey, and testing of proficiency samples in a comprehensive examination to determine a laboratory's capability to perform specific tests. NVLAP, an interactive system between laboratory and accreditor, provides a mechanism for overall laboratory improvement.

501,315
PB86-139912 Not available NTIS
 National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Fields Div.
Review of Electromagnetic Compatibility/Interference Measurement Methodologies.
 Final rept.,
 M. T. Ma, M. Kanda, M. L. Crawford, and E. B. Larsen. 1985, 24p
 Pub. in Proceedings of IEEE, v73 n3 p388-411 Mar 85.

Keywords: *Electromagnetic interference, *Electromagnetic compatibility, Measurement, Electric devices, Reprints.

The paper presents a review summary of radiated emission and susceptibility measurement methodologies currently used for assessing the electromagnetic compatibility/interference (EMC/EMI) characteristics of electronic devices and systems. In particular, measurement methods using open sites, transverse electromagnetic (TEM) cells, reverberating chambers, and anechoic chambers are discussed, in light of their technical justifications and bases, their strengths and limitations, and interpretation of the measured results.

501,316
PB86-139946 Not available NTIS
 National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Fields Div.
EMI (Electromagnetic Interference) Measurement Challenge.
 Final rept.,
 C. K. S. Miller. 1983, 9p
 Pub. in Proceedings of Measurement Science Conference (1983), Accuracy and Automation, Palo Alto, California, January 20-21, 1983, p189-197.

Keywords: *Electromagnetic interference, Measurement, Electromagnetic environments, Electromagnetic radiation, Electromagnetic compatibility.

With the increasing proliferation of radiating sources to the electromagnetic (EM) environment and the increased use of semiconductor technology in consumer and industrial products, incidents of electromagnetic interference (EMI) to electronic products have increased. Current EMI measurement difficulties are reviewed and a description is given of the National Bureau of Standards' (NBS) measurement research, both planned and in process.

501,317
PB86-140001 Not available NTIS
 National Bureau of Standards (NEL), Gaithersburg, MD. Electrosystems Div.
Efficient Calibration Strategy for Linear, Time Invariant Systems.
 Final rept.,
 G. N. Stenbakken, T. M. Souders, and J. A. Lechner. 1984, 1p
 Pub. in Proceedings of Conference on Precision Electromagnetic Measurements, Delft, The Netherlands, August 20-24, 1984, p215.

Keywords: *Frequency response, *Calibrating, Linear systems, Regression analysis, Optimization, Tests, Time invariant systems.

An efficient strategy for accurately characterizing the frequency response of linear, time invariant (LTI) systems is presented. The approach, based on circuit modeling, design-of-experiments theory, and nonlinear regression analysis, optimizes calibration confidence with respect to test effort. The analytical tools and methodology needed for designing the strategy will be included, together with experimental results. The approach can be particularly beneficial in volume testing of instruments such as oscilloscopes, precision ac voltmeters, waveform recorders, and wideband wattmeters.

501,318
PB86-140043 PC A15/MF A01
 National Bureau of Standards (NML), Gaithersburg, MD. Center for Basic Standards.
Technical Activities 1985, Center for Basic Standards.
 K. G. Kessler. Oct 85, 331p NBSIR-85/3254
 See also PB86-121597.

Keywords: *Research, *Standards, Metrology, Fundamental constants, Pressure, Vacuum, Electrical measurement, Temperature, Atomic physics, Mass, Length, Time standards, Frequency standards, Gravity, X rays, Gamma rays, Laser applications.

The report summarizes the research and technical activities of the Center for Basic Standards during the Fiscal Year 1985. These activities include work in the areas of electricity, temperature and pressure, mass and length, time and frequency, quantum metrology, and quantum physics.

501,319
PB86-140209 Not available NTIS
 National Bureau of Standards (NML), Boulder, CO. Time and Frequency Div.
Special Applications.
 Final rept.,
 F. L. Walls, and J. J. Gagnepain. 1984, 10p
 Pub. in Precision Frequency Control, v2 ch15 p287-296 1984.

Keywords: *Quartz resonators, *Frequency measurement, Microbalances, Monitors, Deposition, Pressure sensors, Temperature measuring instruments, Accelerometers, Vibration meters.

The high resolution achievable with frequency metrology often makes it attractive to connect the measurement of physical parameters to a frequency measurement via a suitable transducer. Quartz crystal resonators are sensitive to mass loading and via nonlinear effects, to temperature and stress. The sensitivities are generally low; however, the excellent short-term stability of precision quartz resonators makes high-resolution measurements of temperature, pressure, vibration, acceleration, film thickness, some gas-phase chemical rates, and absorption feasible.

501,320
PB86-140217 Not available NTIS
 National Bureau of Standards (NML), Boulder, CO. Time and Frequency Div.
Other Means for Precision Frequency Control.
 Final rept.,
 F. L. Walls. 1985, 11p
 Pub. in Precision Frequency Control, v2 ch14 p275-285 1985.

Keywords: *Frequency control, Frequency stability, Tuning forks, Resonators, Quartz, Precision, Superconducting cavity resonators.

The chapter outlines the use of quartz tuning forks, high Q LC resonator strip line resonators, superconducting cavities, and dielectrically loaded cavities for precision frequency control. General noise considerations, practical limitations, as well as potential future uses and developments are indicated.

501,321
PB86-140233 Not available NTIS
 National Bureau of Standards (NML), Boulder, CO. Time and Frequency Div.
Frequency and Time, Their Measurement and Characterization.
 Final rept.,
 S. R. Stein. 1985, 42p
 Pub. in Precision Frequency Control, v2 ch12 p191-232 1985.

Keywords: *Frequency measurement, *Time measurement, Frequency stability, Atomic clocks, Spectrum analysis, Computer applications.

The document is chapter 12 in the forthcoming book entitled 'Precision Frequency Control' edited by A. Balato and E. A. Gerber. The book contains contributions from twenty-three authors and an extensive bibliography. Chapter 12 presents the theory and practice of the measurement of frequency and time. Rather than a review of the literature, it is a summary of the best techniques developed during the past twenty-five years. Modern techniques made possible by the proliferation of minicomputers and digital equipment are stressed.

501,322
PB86-140290 Not available NTIS
 National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Fields Div.
Current NBS (National Bureau of Standards) Metrology Capabilities and Limitations at Millimeter Wave Frequencies.
 Final rept.,
 G. R. Reeve, and C. K. S. Miller. 1985, 19p
 Pub. in Proceedings of the Measurement Science Conference (1985), Santa Clara, California, January 17-18, 1985, p296-314.

Field 14—METHODS AND EQUIPMENT

Group 14B—Laboratories, Test Facilities, and Test Equipment

Keywords: *Meteorology, Measuring instruments, Low frequencies, Millimeter waves, Measurement.

It is the intent of the paper to describe the technical demands of responding to the challenges of millimeter-wave technology. A description of the current capabilities that exist at NBS will be given for those parameters and frequencies where measurement services exist. Where novel standards have been developed. Limitations in services and in concepts of standards for providing those services will be described to indicate the degree of research that must be undertaken to satisfy future industrial needs in this evolving technology.

501,323
PB86-142411 Not available NTIS
National Bureau of Standards (NEL), Boulder, CO.
Electromagnetic Technology Div.

Scratch Standard Is Not a Performance Standard.
Final rept.,
M. Young. 1985, 2p
Pub. in Proceedings of Optical Fabrication and Testing Workshop, Cherry Hill, NJ., June 12-13, 1985, pTHAA4-1-THAA4-2.

Keywords: *Standards, *Surfaces, *Optical tests, Scratches, *Scratch standards, Cosmetic standards, MIL standards.

The history and description of the scratch standard is given showing that the scratch number should never be related to its width, and that the standard is cosmetic only.

501,324
PB86-142429 Not available NTIS
National Bureau of Standards (NEL), Boulder, CO.
Electromagnetic Technology Div.

Tunable Scratch Standards.
Final rept.,
M. Young, E. G. Johnson, and R. Goldgraben. 1985, 8p
Sponsored by Department of Defense, Washington, DC.
Pub. in Proceedings of SPIE Measurement and Effects of Surface Defects and Quality of Polish, Los Angeles, CA., January 21-22, 1985, p70-77.

Keywords: *Standards, *Surfaces, *Optical tests, Scratches, *Scratch standards, Cosmetic standards, MIL standards.

The scratch standard (MIL-O-13830A) is a cosmetic standard that is effected by a visual comparison with a set of submasters that is in turn evaluated by comparison with a set of master standards. Both manufacture and certification of the submasters are somewhat unreliable. In the paper, the authors show that the submasters can be classified according to the relative power scattered at a relatively small angle. They have designed etched gratings with which to replace the submasters; these gratings have the appearance of scratches but diffract a broad peak between 5 and 10 degrees off the axis of the incident beam. They have classified some prototypes both by comparison with the master standards and by a photoelectric measurement; agreement between the two methods is good. The authors suggest that such gratings be used as the submasters and possibly that they be classified by a photoelectric rather than visual measurement.

501,325
PB86-142700 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Electrosystems Div.

Efficient Calibration Strategies for Linear, Time Invariant Systems.
Final rept.,
G. N. Stenbakken, T. M. Souders, J. A. Lechner, and P. T. Boggs. 1985, 6p
Pub. in Proceedings of Autotestcon '85 IEEE International Automatic Testing Conference, Uniondale, NY., October 22-24, 1985, p361-366.

Keywords: *Frequency response, *Calibrating, Linear systems, Tests, Time invariant systems, Parameter estimation.

An efficient strategy for accurately characterizing the frequency response of linear, time invariant systems is presented. The approach, based on circuit modeling, test point selection, and parameter estimation, optimizes calibration confidence with respect to test effort. The analytic tools and methodology needed for designing the strategy are included, together with experi-

mental results. The approach can be particularly beneficial in volume testing of devices such as amplifiers, attenuators and filters, or systems whose frequency response is dominated by such devices.

501,326
PB86-142874 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.

Comparison of Sputtered Ni/Cr Interface Depth Resolution as Obtained by the Quartz Crystal Microbalance Mass-Loss Method and Auger Spectroscopy.
Final rept.,
B. Navinsek, P. Panjan, A. Zabkar, and J. Fine. 1985, 3p
Pub. in Jnl. of Vacuum Science and Technology A3, n3 p671-673 May/Jun 85.

Keywords: *Interfaces, *Depth finding, Nickel, Chromium, Microbalances, Quartz, Sputtering, Metal films, Thin films, Comparison, Reprints, Auger electron spectroscopy.

Sputter depth profiles of interfaces have been obtained by monitoring the change in sputtering rate as a function of sputtered depth. One very sensitive technique which we use to measure sputtering rates is the quartz crystal microbalance mass-loss method; it has been used to characterize Ni/Cr interfaces sputtered with a mass-analyzed 6 to 12 keV argon ion beam. Interface widths or interface depth resolution (90 to 10% points) obtained from the mass-loss depth profile data are compared to Auger sputter depth profile widths (1 to 4.5 keV argon ions) obtained on similar Ni/Cr thin-film materials. The somewhat narrower widths found with the mass-loss method indicate that this type of depth profiling can be used to characterize interface structures and to estimate the abruptness of an original, unsputtered interface.

501,327
PB86-143732 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Semiconductor Materials and Processes Div.
Practical Method for Edge Detection and Focusing for Linewidth Measurements on Wafers.
Final rept.,
D. Nyssonen. 1985, 7p
Pub. in SPIE Optical Microlithography IV 538, p172-178 1985.

Keywords: *Line width, *Optical measurement, *Dimensional measurement, *Lithography, Optical microscopes, Focusing, Wafers, Micrometers, Reprints, *Edge detection.

Lack of precision and accuracy of in-process critical dimension (CD) measurements of linewidth continues to be a serious problem at micrometer and submicrometer dimensions. The paper proposes a new dual-threshold method for edge detection and focusing, based on image theory, which can be adapted to most optical microscope-based measurement systems. It does not require knowledge of the phase difference at the line edge. The accuracy of this criterion is compared to two more widely used criteria, (1) the minimum and (2) 50% threshold, and it is concluded that, when the phase difference is unknown and varies with normal processing, the new dual-threshold method is the superior method.

501,328
PB86-144136 PC A99/MF E04
National Bureau of Standards (NML), Gaithersburg, MD. Center for Basic Standards.

Precision Measurement and Calibration: Electricity. Selected Papers on the Realization and Maintenance of the Fundamental Electrical Units and Related Topics.
Final rept.,
A. O. McCoubrey. Oct 85, 860p NBS/SP-705
See also N70-31104. Library of Congress catalog card no. 85-600580.

Keywords: *Electricity, Units of measurement, Electrical measurement, Calibrating, Electromagnetism, Quantum electronics.

The present volume in the field of electricity, includes 66 more recent papers by NBS authors and 16 abstracts of closely related papers by authors from other organizations. In view of the expansion of measurement technologies used in electricity and electromagnetism it has been necessary to reduce the range of topics for the selection of papers in the new compila-

tion. In the connection an emphasis has been placed upon the realization and maintenance of fundamental electrical units and the related scientific advances, particularly in quantum physics. However, in the interest of completeness, three appendices also provide up-to-date bibliographies of publications by NBS authors in different areas of electromagnetism.

501,329
PB86-150232 PC A12/MF A01
National Bureau of Standards, Gaithersburg, MD.
National Conference on Weights and Measures (70th), 1985.
Final rept.,
A. D. Tholen, L. E. Barbrow, and A. P. Heffernan. Nov 85, 267p NBS/SP-704
See also PB85-178432. Library of Congress catalog card no. 26-27766.

Keywords: *Metrology, *Meetings, Weight measurement, Metric system, Standards, Measurement.

These are the proceedings of the 70th Annual Meeting of the National Conference on Weights and Measures. Reports by the several standing and annual committees of the Conference comprise the major portion of the publication. Included also are papers presented by Conference officials and others. Major issues discussed at the Conference included a new Scales Code to be effective January 1, 1986, method of sale of commodities, labeling of gasoline-alcohol blends, national type evaluation, and development of training materials.

501,330
PB86-154077 PC A04/MF A01
National Bureau of Standards, Gaithersburg, MD. Office of Product Standards Policy.
Self-Evaluative Laboratory Quality System,
C. J. Kelly, K. D. Bruley, D. H. Craig, D. J. Pangonis, and J. W. Locke. Nov 85, 64p NBSIR-85/3278
Prepared in cooperation with Ford Motor Co., Dearborn, MI.

Keywords: *Laboratories, *Quality assurance, Quality control, Measurement, Systems analysis.

The report describes the evaluation of Measurement Assurance Experiments (MAEs) for determining the quality of within-laboratory test data. A general self-evaluative quality system is outlined and objective measures of data quality, precision and/or accuracy are presented for four fully described MAEs. Measurement Assurance Programs (MAPs), laboratory accreditation, and internal quality audits are also discussed.

501,331
PB86-162179 PC A04/MF A01
National Bureau of Standards (NEL), Gaithersburg, MD. Robot Systems Div.
Measurement Technology for Automation in Construction and Large Scale Assembly,
J. M. Evans. Aug 85, 67p NBSIR-85/3310
Proceedings of a workshop held at Washington, DC. on February 5-6, 1985. Sponsored by Transitions Research Corp., Hartford, CT.

Keywords: *Metrology, Automation, Construction, Robots, Assembling, Technology, Numerical control.

The workshop, sponsored by the National Bureau of Standards and Transitions Research Corporation, concluded that: New technology achievable in the near term would have a major benefit in the construction and large scale assembly industries. The key to this benefit is the application of computers to data management and process control both off-site for design and planning and on-site for inventory management, production control and creation of an as-built data base. The achievement of this new technology requires research carried out on the integration of systems for measurement and automated control of on-site construction and assembly tasks.

501,332
PB86-165867 (Order as PB86-165776, PC A08/MF A01)
Amsterdam Univ. (Netherlands).
Use of Kalman Filtering and Correlation Techniques in Analytical Calibration Procedures,
H. C. Smit. 24 Jun 85, 11p
Sponsored by National Bureau of Standards, Gaithersburg, MD.

Included in Jnl. of Research of the National Bureau of Standards, v90 n6 p441-451 Nov-Dec 85.

Keywords: *Chemical analysis, *Calibrating, Laboratory equipment, Correlation techniques, *Kalman filtering, *Chemometrics, Computer applications, Procedures.

Different chemometric methods to improve calibrations are described. A Kalman filter is applied for processing and predicting slowly varying parameters of a linear calibration graph. The results are used for the evaluation of unknown samples, and for deciding whether to calibrate again or to analyze the next unknown sample. Another approach of the calibration problem, particularly in chromatography, is the use of correlation techniques. The noise reduction property of correlation chromatography is used to extend the calibration graph to very low concentrations. Furthermore, an experimental technique to determine a calibration curve and the unknown sample simultaneously under exactly the same conditions is described.

501,333
PB86-165875

(Order as PB86-165776, PC A08/MF A01)
Texas Univ. at El Paso.
Intelligent Instrumentation,
A. M. Harper, and S. A. Liebman. 1 Jul 85, 12p
Prepared in cooperation with Aberdeen Proving Ground, MD. Sponsored by National Bureau of Standards, Gaithersburg, MD.
Included in Jnl. of Research of the National Bureau of Standards, v90 n6 p453-464 Nov-Dec 85.

Keywords: *Laboratory equipment, Feasibility studies, Statistical analysis, Gas chromatography, Mass chromatography, Pattern recognition, Pyrolysis, Expert systems, Computer applications.

Three areas of modern analysis will be discussed: (1) developments in the area of preprocessing and pattern recognition systems of pyrolysis gas chromatography and pyrolysis mass spectrometry; (2) methods projected for the cross interpretation of several analysis techniques such as several spectroscopies on single samples; and (3) the advantages of having well defined chemical problems for expert systems/pattern recognition automation.

501,334
PB86-165891

(Order as PB86-165776, PC A08/MF A01)
Houston Univ., TX.
Optimization,
S. N. Deming. 1 Jul 85, 6p
Sponsored by National Bureau of Standards, Gaithersburg, MD.
Included in Jnl. of Research of the National Bureau of Standards, v90 n6 p479-485 Nov-Dec 85.

Keywords: *Experimental design, *Chemical analysis, *Optimization, Mathematical models, Screening.

Most research and development projects require the optimization of a system response as a function of several experimental factors. Familiar chemical examples are the maximization of product yield as a function of reaction time and temperature; the maximization of analytical sensitivity of a wet chemical method as a function of reactant concentration, pH, and detector wavelength; and the minimization of undesirable impurities in a pharmaceutical preparation as a function of numerous process variables. The 'classical' approach to research and development involves answering the following three questions in sequence: What are the important factors (Screening), In what way to these important factors affect the system, (Modeling), What are the optimum levels of the important factors. As R. M. Driver has pointed out, when the goal of research and development is optimization, an alternative strategy is often more efficient: What is the optimum combination of all factors levels, (Optimization), In what way do these factors affect the system, (Modeling in the region of the optimum), What are the important factors. The key to this alternative approach is the use of an efficient experimental design strategy that can optimize a relatively large number of factors in a small number of experiments. The theory of these techniques and applications to real situations will be discussed.

501,335
PB86-166725
National Bureau of Standards (NEL), Boulder, CO.
Electromagnetic Fields Div.

Finline Diode Six-Port: Fundamentals and Design Information,
M. Weidman. Dec 85, 43p NBS/TN-1090
Also available from Supt. of Docs as SN003-003-02714-6.

Keywords: Network analyzers, Millimeter waves, Integrated circuits, Planar devices, Design, *Six ports.

The preliminary design and testing of a planar circuit six-port with diode detectors is described. The planar circuit medium was chosen to be finline, and all preliminary work was done in WR-42 waveguide (18-26.5 GHz). The finline substrate was alumina, and initially commercial beam-lead diodes were bonded to the finline metalization. The goal is to design an integrated circuit which could be fabricated on one chip (with diode detectors) and used as part of a six-port network analyzer in the waveguide bands above 18 GHz. Initial designs proved to be unsatisfactory because of high losses and reflections. Most of the problems have been solved, and a usable integrated finline circuit is a good possibility for a millimeter wave six-port.

501,336
PB86-166782
National Bureau of Standards, Gaithersburg, MD.
Journal of Research of the National Bureau of Standards, Volume 90, Number 5, September-October 1985.
Oct 85, 64p
See also PB86-166790 through PB86-166832. and PB86-137627. Also available from Supt. of Docs SN703-027-00006-7. Library of Congress catalog card no. 63-37059.

Keywords: *Research projects, Thermodynamics, Solutions, Sulfur dioxide, Standards, Speech recognition, Performance evaluation, Automatic control equipment, Weight measurement, Weight indicators, Temperature, Succinonitrile, Assessments, Reaction kinetics, Standard reference materials.

Contents:
Note on Weighings Carried Out on the NBS-2 Balance;
Thermodynamics of Solution of SO₂(g) in Water of Aqueous Sulfur Dioxide Solutions;
SRM 1970:
Succinonitrile Triple-Point Standard-A
Temperature Reference Standard Near 58.08C;
Performance Assessment of Automatic Speech Recognizers;
Chemical Kinetics-Theory and Experiment.

501,337
PB86-166790
(Order as PB86-166782, PC A04/MF A01)
National Bureau of Standards, Gaithersburg, MD.
Note on Weighings Carried Out on the NBS-2 Balance,
R. S. Davis, and P. Carre. 28 Aug 85, 9p
Prepared in cooperation with Bureau International des Poids et Mesures, Sevres (France).
Included in Jnl. of Research of the National Bureau of Standards, v90 n5 p331-339 Sep-Oct 85.

Keywords: *Weight indicators, *Weight measurement, Design criteria, Performance evaluation.

The NBS-2 balance was designed and built at NBS and transferred to the BIPM in 1972. It is presently used for the comparison of national prototype kilograms with international standards. Excellent environmental conditions at the BIPM have resulted in a long-term standard deviation of 1 microgram (1 x 10 to the -9th power) for a comparison of two 1-kilogram standards. With this remarkable precision, one has begun to observe and quantify systematic biases of less than 5 micrograms. The nature of these biases is presented as well as the remedy adopted to eliminate their influence on both the final measurement results and the variance assigned to those results.

501,338
PB86-166816
(Order as PB86-166782, PC A04/MF A01)
National Bureau of Standards, Gaithersburg, MD.
SRM 1970: Succinonitrile Triple-Point Standard - A Temperature Reference Standard Near 58.08C,
B. W. Mangum, and S. El-Sabban. 8 Aug 85, 12p
Prepared in cooperation with National Inst. for Standards, Cairo (Egypt).
Included in Jnl. of Research of the National Bureau of Standards, v90 n5 p359-370 Sep-Oct 85.

Keywords: *Succinonitrile, *Thermometers, Temperature measurement, Standards, Calibrating, *Standard reference materials.

Triple-point-of-succinonitrile cells have been tested and established as Standard Reference Material (SRM) 1970. Of the 115 cells tested, 109 were accepted as SRM 1970. Five of the 115 cells had triple-point temperatures lower than 58.0785C (the low-temperature limit established for SRM 1970) and, consequently, were rejected. One of the 115 cells broke during tests on it. The mean value of the triple-point temperatures (obtained by freezing) of the 109 cells is 58.0796 + or - 0.0015C, where the uncertainty is the total estimated uncertainty relative to the International Practical Temperature Scale of 1968, Amended Edition of 1975. The standard deviation of the triple-point temperatures is 0.48 mK. The purity of the succinonitrile of the SRM 1970 cells is estimated to range from 99.999.97% to 99.999.84%. The preparation of the cells, the various tests performed on them, and the procedure recommended for their use are described.

14E. Reprography

501,339
PB85-212082
National Bureau of Standards (NML), Gaithersburg, MD. Office of Standard Reference Data.
Contribution to Computer Typesetting Techniques (for Microcomputers).
Data file,
R. C. Thompson. Apr 76, 6 diskettes NBS/DF/DK-85/003
For system on magnetic tape, see PB-263 925, and PB-263 926.
The data file is contained on 5 1/4-inch, double-sided, double-density diskettes, compatible with the IBM-PC microcomputer. The file is in ASCII. New formats will likely be available in the future. Contact NTIS Computer Products for current formats. Price includes documentation, PB-251 845.

Keywords: *Data file, *Plotting, Digital techniques, Fonts, Magnetic tapes, *Alphanumeric symbols, *Graphics, Typesetting, Vector processing, Hershey character set.

The diskettes contain two files. The first file contains tables of coordinates which make it possible to generate 1377 different alphabetic and graphic characters on either COM devices or on digital plotters. The characters can be generated on vector plotters by connecting the points given in these tables. This method of digitizing graphic arts characters allows them to be generated on any device which can plot vectors of arbitrary length and direction. The second file contains the Katakana, Hiragana, and approximately 600 Kanji characters also digitized by Dr. Allen V. Hershey of the Naval Surface Weapons Laboratory in Dahlgren, VA. This particular version of the data file is contained on 5 1/4 in. floppy disks formatted for the IBM PC microcomputer and PC-compatible microcomputers.

17.

NAVIGATION, COMMUNICATIONS, DETECTION, AND COUNTERMEASURES

17B. Communication

501,340
PB85-189363 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg,
MD. Law Enforcement Standards Lab.
Telephone Dialers with Taped Voice Messages.
Final rept.
Oct 84, 18p
Sponsored by National Inst. of Justice, Washington,
DC.
Pub. in NIJ (National Inst. of Justice) Standard-
0322.00, 18p Oct 84.

Keywords: *Warning systems, *Telephone equipment,
Standards, Performance, Voice communication,
*Telephone dialers.

The standard establishes performance requirements
and test methods for evaluating dialers that dial one or
more specified telephone numbers and transmit one or
more taped voice messages in response to an actua-
tion. These devices transmit an alarm signal (the
voice message(s)) through the ordinary switched tele-
phone network to a telephone answering service or
private phone. Emphasis in this standard is on charac-
teristics affecting the ability of the devices to perform
their tasks reliably and on factors that affect false
alarm susceptibility.

501,341
PB85-189371 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg,
MD. Law Enforcement Standards Lab.
Telephone Dialers with Digitally Coded Messages.
Final rept.
Oct 84, 18p
Sponsored by National Inst. of Justice, Washington,
DC.
Pub. in NIJ (National Inst. of Justice) Standard-
0323.00, 18p Oct 84.

Keywords: *Warning systems, *Telephone equipment,
Standards, Performance, Digital systems, *Telephone
dialers.

The standard establishes performance requirements
and test methods for digital dialers. These dialers are
intended to dial one or more preprogrammed tele-
phone numbers and to transmit digitally coded mes-
sages in response to an actuation. These alarm mes-
sages are transmitted to special digital signal receivers
via the ordinary switched telephone network. Empha-
sis in this standard is on characteristics that influence
the ability of the dialer to perform its intended function
reliably and some factors that affect false alarm sus-
ceptibility.

501,342
PB85-196269 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
**GRIDNET - An Alternative Large Distributed Net-
work.**
Final rept.,
R. T. Moore, N. F. Geer, and H. A. Graf. 1984, 10p
Pub. in Computer 17, n4 p57-66 Apr 84.

Keywords: Data links, Routing, Reprints, *Distributed
computer systems, *Communications networks,
Packet switching, Distributed processing.

GRIDNET is a highly connected, highly reliable and
survivable data communications network based on the
use of distributed processing and redundant data links.
Alternate routing of traffic around outages is per-
formed without the use of global operability status in-
formation using only information about the status of
near neighbors. Computer simulation was used to de-
velop estimates of the performance characteristics of
the network.

501,343
PB85-197770 Not available NTIS
National Bureau of Standards (NEL), Boulder, CO.
Electromagnetic Technology Div.
**Use of Power Transfer Matrices in Predicting
System Loss: Theory and Experiment.**
Final rept.,
J. M. Maisonneuve, and R. L. Gallawa. 1984, 6p
Sponsored by Centre de Documentation de l'Arme-
ment, Paris (France). Direction des Recherches,
Etudes et Techniques.
Pub. in Proceedings of SPIE, Fiber Optics: Short-Haul
and Long-Haul Measurements and Applications II, San
Diego, CA., August 21-22, 1984, v500, p88-93.

Keywords: Attenuation, *Local area networks, *Fiber
optics transmission lines, Ray theory, Power transfer.

The phase space diagram for parabolic and step index
fibers leads to a graphic representation of the bound,
leaky, and refracted rays of ray theory. This concept is
used to predict the attenuation of typical components
of local area networks. The technique uses power
transfer matrices to track the evolution of power distri-
bution in ray packets. In particular, we predict and then
measure the power transfer of two ray packets for a
step index fiber. The comparison is encouraging.

501,344
PB85-202083 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Measuring a Local Network's Performance.
Final rept.,
P. D. Amer, R. Rosenthal, and R. E. Toense. 1983,
10p
Pub. in Data Commun. 12, n4 p173-182 Apr 83.

Keywords: *Computer networks, *Communication net-
works, *Radio broadcasting, Traffic, Evaluation, Meas-
urement, Performance, Computer systems hardware,
Reprints, *Local area networks, Multichannel commu-
nications, Multiple access, NBSNET network, Comput-
er software.

A local area computer network (LAN) measurement
center has been implemented at the National Bureau
of Standards, Institute for Computer Sciences and
Technology (ICST) for the performance investigation
of NBSNET, one of the largest operational local broad-
cast networks. The measurement center is a facility for
characterizing NBSNET traffic and for performing re-
search experiments with artificially generated traffic.
The center consists of four components: a monitoring
system for collecting measurements about both arti-
ficial and normal network traffic, an artificial traffic gen-
erator for emulating various loads on the network,
analysis software for summarizing the measurement
information into performance reports, and a develop-
ment system for generating hardware and software
support of the entire measurement center. A taxonomy
of audiences interested in local network traffic charac-
terization is presented.

501,345
PB85-221919 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Performance Analysis of NBSNET.
Final rept.,
R. E. Toense. 1983, 10p
Pub. in Jnl. Telecommun. Networks 2, n2 p177-186
1983.

Keywords: *Computer networks, *Telecommunication,
Carriers, Performance evaluation, Utilization, Channel
stabilization, Reprints, *Communications networks,
*Local area network, NBSNET, NBS network, Broad-
casting.

The performance of NBSNET, a broadcast, packet
switched, carrier sense multiple access with collision
detection (CSMA/CD) local area network, is analyzed
in terms of utilization, stability, delay and fairness. Traf-
fic generators transmit packets of known arrival rate
and packet length distributions on an isolated network
segment. The packets are recorded and time-stamped
for analysis. Analysis of the empirical laboratory data

shows that (1) utilization of the network under heavy
and overloaded conditions approaches the theoretical
limit and is predictable, (2) the network remains stable
under the conditions observed, (3) the mean delay in-
troduced by the network is predictable as a hyperbolic
function of the observed channel utilization, (4) the
network is fair with uniformly distributed individual
node utilizations.

501,346
PB85-222271 Not available NTIS
Bolt Beranek and Newman, Inc., Cambridge, MA.
Design of a Message Format Standard.
Final rept.,
D. Deutsch. 1981, 22p
Contract NB79-SBCA-0092
Pub. in Proceedings of IFIP TC-6 Int. Symp. Computer
Message Systems, Ottawa, Canada, April 6-8, 1981,
p199-220.

Keywords: Standards, Design, Computer systems
hardware, Data links, *Message processing, *Mes-
sage formats, *Computer communications, Office
management, Electronic mail.

Computer Based Message Systems (CBMS), once ex-
clusive tools of programmers and researchers, are
rapidly finding their way into commercial and govern-
mental offices. The first CBMSs were designed as
closed systems, allowing messages to be exchanged
only between the users of the same CBMS. The prolif-
eration of CBMSs has been accompanied by a growing
desire by users for communication between different
systems. Standards and protocols provide common
ground for the interconnection of dissimilar systems.
The paper discusses the design and rationale of a
draft CBMS message format standard being devel-
oped by Bolt Beranek and Newman under contract to
the U.S. National Bureau of Standards. The draft
standard provides a machine-readable format for the
representation of CBMS messages as they are sent or
received by computer based mail systems. It also pro-
vides a set of standard message fields which may be
used to convey specific information often found in
CBMS messages.

501,347
PB86-105277 PC A03/MF A01
National Bureau of Standards (NEL), Boulder, CO.
Center for Electronics and Electrical Engineering.
**Transparent Metrology of Signal to Noise Ratios of
Noisy Band-Limited Digital Signals.**
D. Halford. Jun 85, 32p NBS/TN-1077
Also available from Supt. of Docs SN003-003-02658-
1.

Keywords: *Signal to noise ratio, *Pulse communi-
cation, Metrology, Noise(Sound), Measurement, Moni-
tors, Real time operations, Signals, Synchronism.

The author propose the use of a template method for
quantitative, correct, and transparent measurement of
signal power to additive noise power ratios (SNR) of
digital signals and systems under full operating condi-
tions. The author discusses the significance of trans-
parent metrology, the measurement of various SNR's
by the template method, and the general applicability
of the template method for measurements on any
noisy digital signal. The template method can provide
transparent metrology procedures for other basic meas-
urands, e.g., intersymbol interference, multiplicative
noises, and synchronization.

501,348
PB86-133410 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Internetwork Protocol.
Final rept.,
R. Callon. 1983, 6p
Pub. in Proceedings of IEEE (Institute of Electrical and
Electronics Engineers) 71, n12 p1388-1393 1983.

Keywords: *Computer networks, Telecommunication,
Reprints, Protocols.

Application of the OSI protocols to the 'real world' re-
quires cost-effective interconnection of a wide variety
of existing and future networks. Differences in underly-
ing technologies, in administrative control, in available
qualities of service, and in other important factors
complicate the task of achieving interconnection. The
paper discusses a variety of the major technical issues
related to achieving interconnection within the OSI
network layer.

501,349
PB86-146537 CP T03
 National Bureau of Standards, Gaithersburg, MD. Inst. for Computer Sciences and Technology.
NBS/OSI (National Bureau of Standards/Open Systems Interconnection) Transport Class 4.
 Software,
 D. E. Rorrer, and M. A. Wallace. Oct 85, mag tape
 NBS/SW/MT-86/002
 Supersedes PB84-222918.
 Source tape is in the ASCII character set. This restricts preparation to 9 track, one-half inch tape only. Identify recording mode by specifying density only. Call NTIS Computer Products if you have questions. Documentation is included on the tape.

Keywords: *Software, *Telecommunication, *Data transmission, Operating systems(Computers), Standards, Magnetic tapes, *Transport class 4, C programming language, DEC VAX 11-780 Computers, EUNICE/VMS V3.7 operating systems.

The tape consists of programs which provide the NBS implementation of OSI Transport Class 4 and a test system which measures the conformance of an implementation to the ISO standard. It was written 'c' language and developed under 'EUNICE', a UNIX simulator running on the VMS V3.7 operating system. Also, the Transport implementation uses an interprocess communication facility composed of port, await, and capac system manipulation routines, an internal timer facility and specialized string handling functions. Documentation on the implementation and test system is included on tape...Software Description: The program is written in the C programming language for implementation on a DEC VAX 11-780 computer using the EUNICE/VMS V3.7 operating system.

501,350
PB86-166824
 (Order as PB86-166782, PC A04/MF A01)
 National Bureau of Standards, Gaithersburg, MD.
Performance Assessment of Automatic Speech Recognizers.
 D. S. Paillett. 3 Sep 85, 17p
 Included in Jnl. of Research of the National Bureau of Standards, v90 n5 p371-387 Sep-Oct 85.

Keywords: *Speech recognition, Automation, Signal processing.

The paper discusses the factors known to influence the performance of automatic speech recognizers and describes test procedures for characterizing their performance. It is directed toward all the stakeholders in the speech community (researchers, vendors and users) consequently, the discussion of test procedures is not directed toward the needs of specific users to demonstrate the performance characteristics of any one specific algorithmic approach or particular product. It relies significantly on contributions from an emerging consensus standards activity, especially material developed within the IEEE Working Group on Speech I/O Performance Assessment.

17G. Navigation and Guidance

501,351
PB85-228393 PC A09/MF A01
 National Bureau of Standards (NBS), Boulder, CO. Electromagnetic Technology Div.
VOR (Very-High-Frequency Omnidirectional Range) Calibration Services.
 N. T. Larsen, D. F. Vecchia, and G. R. Sugar. Apr 85, 179p NBS-TN-1069
 Also available from Supt. of Docs as SN003-003-02652-2.

Keywords: *Radio beacons, *Calibrating, VOR(Very high frequency omnidirectional radio range).

The National Bureau of Standards has designed, constructed, and evaluated a standard for the support of very-high-frequency omnidirectional range (VOR) air navigation aids. The standard consists of two instruments: (1) a digital waveform signal generator for the composite VOR audio waveform, and (2) a standard phasemeter based on time series analysis of the waveform. Experimental results, a statistical analysis of them, and the principal software listings are included.

501,352
PB86-129046 Not available NTIS
 National Bureau of Standards (NML), Boulder, CO. Time and Frequency Div.
Simplified GPS C/A Receiver Front End with Low Noise Performance.
 Final rept.,
 D. D. Davis, and A. D. J. Clements. 1985, 8p
 Pub. in Proceedings of Annual Precise Time and Time Interval Applications and Planning Meeting (16th), Greenbelt, MD., November 27-29, 1984, p467-474 1985.

Keywords: *Receivers, Antennas, *Down-converters, *Multipliers, Low noise, Global positioning system.

A redesign of the antenna electronics package for the NBS/GPS C/A receiver has resulted in significantly reduced cost and improved performance. Major improvements include a simplified and more reliable multiplier/mixer, elimination of all twelve piston trimmer tuning capacitors in the original design, elimination of expensive bandpass filters, less expensive antenna and a simplified packaging scheme.

501,353
PB86-138617 Not available NTIS
 National Bureau of Standards (NML), Boulder, CO. Time and Frequency Div.
Global Positioning System for Accurate Time and Frequency Transfer and for Cost-Effective Civilian Navigation.
 Final rept.,
 J. L. Jespersen, M. Weiss, D. D. Davis, and D. W. Allan. 1980, 1p
 Pub. in Proceedings of IEEE Plans 80, Position Location and Navigation Symposium, Atlantic City, New Jersey, December 8-11 1980, p468.

Keywords: *Navigation, Position(Location), Time, Frequencies, Atomic clocks, *Global positioning system.

The paper described some alternative applications of Global Positioning System (GPS) including a method for very accurate time transfer and for civilian position location much less expensively than the designed Department of Defense method. The first part of the paper discusses several time transfer techniques with emphasis on what we call the 'common-view' approach, and the second part considers the system for position location. Both applications depend on the fact that accurate ephemerides are available for GPS and that GPS time is based on atomic clocks.



18.

NUCLEAR SCIENCE AND TECHNOLOGY

18A. Fusion Devices (Thermonuclear)

501,354
PB85-196129 Not available NTIS
 National Bureau of Standards, Gaithersburg, MD.
Perturbation of the Composition Depth Profile of a Material Due to Multi-Directional Ion Bombardment.
 Final rept.,
 O. F. Goktepe, M. J. Roush, F. Davarva, and T. D. Andreadis. 1982, 2p
 Sponsored by American Nuclear Society, LaGrange Park, IL.
 Pub. in Transactions of the American Nuclear Society 1982 Winter Meeting, Washington, DC., November 14-18, 1982, v43 p190-191.

Keywords: *Radiation damage, Ion beams, Monte Carlo method, Xenon, *Ion bombardment, *First wall, *Fusion reactors, EVOLVE computer program.

The ion bombardment of multi-element solids, whether in alloy or oxide form, often leads to marked compositional changes at the surface as a consequence of ion implantation, preferential sputtering, and atomic cascade mixing. For fixed energy ions, these mechanisms produce a composition profile which is dependent upon the incident angle of the ions. Research in the area of ion-bombardment-induced composition changes has almost exclusively dealt with mono-directional ion beams. Most applications of ion bombardment are concerned with well-collimated beams. In the case of the first wall of a fusion reactor, however, the impinging ions are not restricted to any particular angle. The Monte Carlo code EVOLVE, which models the ion bombardment of surfaces, has been used to correlate the composition changes due to a multidirectional ion beam to those of mono-directional beams. Calculations are presented for a multi-directional Xe beam of 1.5 keV containing equal portions of ions with incident angles of 0 degrees and 70 degrees.

501,355
PB85-236362 PC A15/MF A01
 National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.
Materials Studies for Magnetic Fusion Energy Applications at Low Temperatures - 8.
 Technical rept.,
 R. P. Reed. May 85, 335p NBSIR-85/3025
 See also PB84-217488. Sponsored by Department of Energy, Washington, DC. Office of Fusion Energy.

Keywords: *Superconducting magnets, *Stainless steels, *Composite materials, *Cryogenics, Mechanical properties, Weldments, Materials, Technology transfer, Magnetic fusion energy, Steel 304, Steel 14Mn 1Mo 8Ni, Carbon reinforced plastics, Steel 18 Cr 13Mn 3Ni.

The report contains results of a research program to produce material property data that will facilitate design and development of cryogenic structures for the superconducting magnets of magnetic fusion energy power plants and prototypes. The program was developed jointly by the staffs of the National Bureau of Standards and the Office of Fusion Energy of the Department of Energy; it is managed by NBS and sponsored by DOE. Research is conducted at NBS and at various other laboratories through subcontracts with NBS. Research results for 1984 are summarized in an initial 'Highlights of Results' section and reported in detail in the technical papers that form the main body of this report. The technical papers are presented under four headings reflecting the main program areas: Welding, Nonmetallics, Structural Alloys, and Technology Transfer. Objectives, approaches, and achievements are summarized in an Introduction to each program area.

18B. Isotopes

501,356
PB85-197606 Not available NTIS
 National Bureau of Standards, Gaithersburg, MD.
Calibration for Measurements with Background Correction Applied to Uranium-235 Enrichment.
 Final rept.,
 W. Liggett. 1983, 16p

Pub. in Nuclear Instruments and Methods in Physics Research 216, n3 p455-570 1 Nov 83.

Keywords: *Uranium 235, *Enrichment, *Calibrating, *Gamma ray spectroscopy, Reprints.

In enrichment measurement by gamma spectroscopy, two activity levels are observed: One is the sum of the response to the enrichment and a background level, and the second is another background level. Calibration consists of determining not only the relation between the response and the enrichment but also the relation between the two background levels. A calibration procedure with this property is developed under the assumption that the random errors have constant variance and the assumption that the two background levels are proportional. This procedure provides a consistent estimator for the calibration curve and interval estimates for the unknowns measured after calibration. The calibration procedure is applied to enrichment measurements made with the SAM-2 enrichment meter. With these measurements as illustrations, tech-

Field 18—NUCLEAR SCIENCE AND TECHNOLOGY

Group 18B—Isotopes

niques for judging the validity of the assumptions are presented.

501,357

PB85-222313 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Inorganic Analytical Research Div.

Mass Spectrometric Analysis of Uranium and Plutonium Loaded Anion Exchange Resin Beads: An Interlaboratory Round Robin.

Final rept.,
J. D. Fassett, and W. R. Kelly. 1982, 8p
Pub. in Proceedings of ORNL Conf. Analytical Chemistry in Energy Technology, Gatlinburg, TN., 1981, p131-138 1982.

Keywords: *Isotope separation, *Anion exchanging, *Laboratory equipment, *Chemical exchange isotope separation, *Uranium isotopes, *Plutonium isotopes, Polymers, Performance evaluation, Radioactive isotopes, Chemical analysis, Error analysis, Spectroscopic analysis, *Thermal ionization mass spectroscopy.

The resin bead sample loading technique in thermal ionization mass spectrometry has been evaluated for the accurate and precise measurement of uranium and plutonium isotopic ratios by means of an interlaboratory analysis program (round robin) sponsored by the National Bureau of Standards (NBS). Nanogram size samples, including both standards and unknowns, were loaded onto anion exchange resin beads and transported to participating laboratories for measurement. Six laboratories or 40 percent of the laboratories identified as having the requisite high sensitivity instrumentation have participated in all phases of the round robin to date. Isotopic fractionation is concluded to be a major source of imprecision and calibration of isotopic fractionation the major source of inaccuracy.

501,358

PB86-140274 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Occupational Health and Safety Div.

National Bureau of Standards Health Physics Radioactive Material Shipment Survey, Packaging, and Labelling Program Under ICAO/IATA and DOT Regulations.

Final rept.,
D. R. Sharp, and L. A. Slaback. Feb 84, 5p
Pub. in Proceedings of the Health Physics Society Mid-year Topical Symposium (17th), Pasco, Washington, February 5-9, 1984, p7.87-7.91.

Keywords: *Packaging, *Marking, Regulations, Transportation, *Radioisotopes, BASIC computer program, US NBS.

NBS routinely ships, both domestically and internationally, many isotopes in small to moderate activities. These shipments are divided about evenly between Limited Quantity and Type-A shipments, with many containing mixtures of isotopes in a variety of combinations. The ICAO/IATA shipping regulations (and the new DoT regulations on their model) specify individual shipping parameters for every isotope, with limited quantity limits that are additionally a function of physical state. The resulting parametric permutations have become so complex that quality control in the shipment of these radioactive packages has become difficult to maintain. The authors have developed a computer program that will guide a person with minimal training in transportation regulations through package surveys and give exact packaging and labelling instructions. The program is a 27K-byte, user-friendly, BASIC program that runs on the Epson-HX20 notebook computer with microcassette drive and 16K memory expansion unit. This small computer is more manageable than the regulation books for which it will be substituted and will be used in our routine radioactive shipments.

18D. Nuclear Instrumentation

501,359

PB85-207058 Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div.

Design of the NBS (National Bureau of Standards) Magnetic Monopole Detectors.

Final rept.,
A. F. Clark, M. W. Cromar, and F. R. Fickett. 1984, 4p
Pub. in Proceedings of Int. Cryogenic Engineering Conf. (10th), Helsinki, Finland, July 31-August 3, 1984, p365-368.

Keywords: Magnetometers, Superconductors, *Squid(Detectors), *Magnetic monopoles.

Several different configurations of magnetic monopole detectors have been built and operated at the National Bureau of Standards. These have been designed based on the following objectives: (1) Study of the noise characteristics; (2) Simplicity and ease of changing configurations; (3) Operation in relatively large magnetic fields; and (4) Optimum detector area. Satisfying these objectives has resulted in several compromises, but also a flexible and useful apparatus for studying the behavior of the SQUID-detector loop combination with particular emphasis on noise sources that can simulate a monopole signal. Several sources of noise and techniques for their elimination are discussed. Data from the spectral analysis of the noise signals are presented.

501,360

PB85-207074 Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div.

Monopole Detector Studies at NBS (National Bureau of Standards).

Final rept.,
F. R. Fickett, M. Cromar, and A. F. Clark. 1984, 4p
Pub. in Proceedings of Monopole 1983, Ann Arbor, MI., October 6-9, 1983, p477-480 1984.

Keywords: Magnetometers, Superconductors, *Squid(Detectors), *Magnetic monopoles, Squid detectors.

The work at the National Bureau of Standards has had three major goals. First, to investigate sources of noise in SQUID-based detector systems and to develop techniques to minimize their disruptive effects. Second, to investigate and identify sources of signals similar in size and signature to those expected from a monopole passage and, again, to eliminate them. Third, to participate in the search for the monopole. To these ends, the authors have constructed and operated a two-coil coincidence system in several configurations for well over 1000 hours. Because their efforts have been concentrated on the investigation of anomalous effects, not many of these hours can be considered as true detector time.

501,361

PB85-221984 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Nuclear Radiation Div.

Dose Conversion Factors and W sub n Values for Infinitesimal Infinite Tissue-Equivalent Ion Chambers in Monoenergetic Neutron Fields from Thermal to 20 MeV.

Final rept.,
B. R. L. Siebert, and J. J. Coyne. 1984, 4p
Pub. in Radiation Protection Dosimetry 9, n3 p215-218 1984.

Keywords: *Ionization chambers, *Dosimetry, Thermal neutrons, Fast neutrons, Reprints, *Neutron dosimetry, *Tissue-equivalent detectors, Tissue-equivalent materials.

In neutron dosimetry it is common practice to use tissue-equivalent (TE) plastic as a wall material and methane based TE filling gas in constructing ionization chambers and proportional counters. As the materials differ in their elemental composition, Fano's theorem cannot be applied, and therefore it is to be expected that the cavity size has an effect on the response of the instrument. In consequence, the dose conversion factor (i.e. ratio of dose in wall to dose in gas) and the (W sub n) value (i.e. ratio of specific energy deposited in the gas to the specific number of ion pairs created) also depend on the size. The paper gives these ratios for infinitesimal and infinite cavities as a function of neutron energy from thermal to 20 MeV. The relevance of the results to microdosimetric measurements is discussed. Formulas are given which relate the quantities to the primary spectra of charged particles produced by neutrons in materials of interest.

501,362

PB85-222354 Not available NTIS

National Bureau of Standards (NML), Gaithersburg, MD. Nuclear Radiation Div.

Investigation of an Experimental Method for the Determination of Dose Equivalent in the ICRU Sphere.

Final rept.,
G. H. Hartmann, J. J. Coyne, A. Morhart, H. Schuhmacher, and H. G. Menzel. 1984, 4p
Sponsored by Commission of the European Communities, Ispra (Italy).
Pub. in Radiation Protection Dosimetry 9, n3 p207-210 1984.

Keywords: Proportional counters, Calibrating, Standards, Dosimetry, Reprints, *Neutron dosimetry, *Dose equivalents, Tissue-equivalent detectors.

An idealized tissue-equivalent proportional counter of infinitesimal size was assumed for the measurement of dose equivalent in the ICRU sphere. The response of the counter to neutrons over a wide energy range in terms of dose equivalent and its sensitivity in mixed radiation fields have been studied by computer calculations. Results are discussed with respect to the applicability of tissue-equivalent proportional counters in establishing an experimental calibration standard for dose equivalent quantities.

501,363

PB85-229904 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.

Measurement of High Doses Near Metal and Ceramic Interfaces.

Final rept.,
W. L. McLaughlin, J. C. Humphreys, M. Farahani, and A. Miller. 1985, 26p
Pub. in Proceedings of the International Symposium on High-Dose Dosimetry, Vienna, Austria, October 8-10, 1984, p109-133 1985.

Keywords: *Dosimetry, Calcium fluorides, Sodium chloride, Lithium fluorides, Polymeric films, Electron beams, Gamma rays, Alkali halides.

Radiochromic dosimeters consisting of leuco dyes dissolved and cast in very thin (5 to 100 micrometer) plastic films have been shown to be accurate and reproducible dosimeters for measuring absorbed doses in the range 1,000 to 1,000,000 Gy. There are also thin, optical-quality ceramic crystals (e.g. LiF, NaCl and CaF₂) having thicknesses about 0.1 to 2 mm that can provide precise absorbed dose readings in the range 100 to 1 billion Gy by spectrophotometric readings of a series of radiation-induced color-center absorption bands. Besides their relatively broad response ranges, these dosimeters have the advantages of being useful in both photon and electron radiation fields, without great losses in accuracy due to rate or temperature dependence. The plastic films are particularly useful for mapping high-resolution dose distributions, such as depth-dose or isodose contours in thin layers, tubing and wire insulation. It has been shown that, by suitable selection of these plastic and crystalline systems, a fairly wide assortment of materials can be simulated in terms of radiation absorption properties over wide photon and electron spectral ranges (0.01 to 10 MeV).

501,364

PB85-230621 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Nuclear Radiation Div.

Practical Guide to Ionization Chamber Dosimetry at the AFRRI (Armed Forces Radiobiology Research Institute) Reactor.

Final rept.,
L. J. Goodman. Mar 85, 42p
Pub. in Armed Forces Radiobiology Research Institute, Bethesda, Maryland, Contract Report 85-1, p1-41 1985.

Keywords: *Ionization chambers, *Dosimetry, *AFRRI reactor, TRIGA type reactors.

The report provides the dosimetrists at the Armed Forces Radiobiology Research Institute with practical guidance on the use of ionization chambers to perform mixed-field dosimetry at the TRIGA Reactor. Experimental techniques, calculational formulas, physical constants, and correction factors are discussed with the emphasis on practice rather than theory in order to provide consistency and long-term continuity to the reactor dosimetry program at AFRRI.

501,365

PB86-112802 Not available NTIS
National Bureau of Standards (NEL), Boulder, CO.
Electromagnetic Technology Div.
NBS (National Bureau of Standards) Magnetic Monopole Detector.
Final rept.,
M. W. Cromar, A. F. Clark, and F. R. Fickett. 1985, 3p
Pub. in IEEE (Institute of Electrical and Electronics Engineers) Transactions on Magnetism MAG-21, n2 p418-420 Mar 85.

Keywords: Reprints, *Magnetic monopoles, SQUID (Detectors), SQUID devices, Magnetic shielding.

The authors have built and operated several inductive type monopole detectors, the present one having three concentric, orthogonal loops operated in coincidence. The area of each loop is 200 sq cm and the cross sectional area of the superconducting shield is 700 sq cm. The detector loops are in a trapped magnetic field of approximately 3 milligauss. The system is mechanically stable and is relatively insensitive to external disturbances, both mechanical and electro-magnetic. The detector is quiet, having a signal-to-noise ratio for monopole detection of approximately 20. The authors have also investigated several sources of noise and spurious signals which might mimic a monopole event.

501,366

PB86-112851 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Nuclear Radiation Div.
Book Review, Advances in Scintillation Counting.
Final rept.,
B. M. Coursey. 1985, 1p
Pub. in International Jnl. of Applied Radiation and Isotopes 36, n4 p331-332 1985.

Keywords: Reprints, *Scintillation counting, Book reviews.

This book contains the edited papers presented at the International Conference on Advances in Scintillation Counting held in Banff in May of 1983. The organizers asked themselves before undertaking this conference whether a book entitled 'Advances in Scintillation Counting' could live up to its promise. It was well that they considered this question because the decade of the 1970s had seen perhaps too many such conferences. There were at least six international conferences on scintillation counting during this time and, as in many instances the same groups presented papers, it was questionable how much real advancement could occur in the diminishing intervals between meetings.

501,367

PB86-124070 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.
Radiation-Induced Color Centers in LiF for Dosimetry at High Absorbed Dose Rates.
Final rept.,
W. L. McLaughlin, A. Miller, S. C. Ellis, A. C. Lucas, and B. M. Kapsar. 1980, 2p
Pub. in Proceedings of International Conference on Solid State Dosimetry (6th), Toulouse, France, April 1-4, 1980, Nuclear Instrumentation Methods 175, n1 p17-18 Sep 80.

Keywords: *Lithium fluorides, *Color centers, *Dosimetry, *Beta dosimetry, Albedo-neutron dosimeters, Gamma dosimetry, Physical radiation effects.

Color centers formed by irradiation of optically clear crystals of pure LiF may be analyzed spectrophotometrically for dosimetry in the absorbed dose range from 100 to 10 to the 7th power grays. Routine monitoring of intense electron beams is an important application. Both (6)LiF and (7)LiF forms are commercially available, and when used with filters as albedo dosimeters in pairs, they provide discrimination of neutron and gamma-ray doses.

501,368

PB86-128220 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Nuclear Radiation Div.

Calibration of the NBS (National Bureau of Standards) Black Neutron Detector at 2.3 MeV Using the Time-Related Associated-Particle Method.

Final rept.,
K. C. Duvall, A. D. Carlson, and O. A. Wasson. 1985, 3p
Pub. in Nuclear Instruments and Methods in Physics Research B10/11, n9 p931-933 1985.

Keywords: *Calibrating, Neutron sources, *Neutron detectors, MeV range 01-10.

A time-correlated associated-particle measurement capability using the D(d,n)(3)He source reaction has been developed at the National Bureau of Standards 3-MV positive-ion Van de Graaff Accelerator Laboratory. The facility has been used to measure the efficiency of the NBS Black Neutron Detector at a neutron energy of 2.3 MeV. The associated (3)He particles are detected at an angle of 45 degrees with respect to the beam axis which is a more forward angle than conventionally employed. The kinematically more energetic (3)He particles detected at the forward angle are readily separated from scattered deuterons at an incident beam energy of 250 keV. The time-correlated coincidence requirement on events detected in the Black Neutron and associated-particle detectors virtually eliminates the need for background corrections to the Black Neutron Detector rate. A result for the efficiency of the Black Neutron Detector at 2.3 MeV has been obtained with an accuracy of about + or - 1% and agrees well with a Monte Carlo calculated value. The measurement extends the usefulness of the Black Neutron Detector as an absolute neutron flux monitor to the higher energy region.

18E. Nuclear Power Plants

501,369

PB85-242196 PC A04/MF A01
National Bureau of Standards, Gaithersburg, MD.
Heat Release Rate Characteristics of Some Combustible Fuel Sources in Nuclear Power Plants.
B. T. Lee. Jul 85, 53p NBSIR-85/3195
Sponsored by Nuclear Regulatory Commission, Washington, DC.

Keywords: *Fire hazards, *Nuclear power plants, Fuels, Fire safety, Fires, Cables(Power lines), Trays, Flammability, Flammable liquids, Ignition, Wood, Fire tests, Refuse, *Heat release rate.

A major risk to a nuclear power plant is the possibility of serious fire. There is a need to know the heat release rate behavior of combustible fuels in the plant in order to help reduce the fire threat to the facilities. Heat release rate characteristics of cable tray fires and some of the associated potential external ignition sources are discussed. Existing correlations are given for determining the time to ignition and the subsequent heat release rate of spills and pools of flammable liquids. Approximate correlations are developed for heat release rate for trash fires as a function of fire size and for one particular cable tray array arrangement as a function of the type of cable. In addition, a scheme is given for calculating the heat release rate from wood fuel fires.

18F. Radiation Shielding and Protection

501,370

PB85-189231 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Nuclear Radiation Div.
Evaluation of Dose Equivalent Per Unit Fluence for a D2O-Moderated 252Cf Neutron Source.
Final rept.,
C. Eisenhauer. 1984, 2p
Pub. in Radiation Protection Dosimetry 9, n1 p63-64 1984.

Keywords: *Neutron sources, Fission neutrons, Dosimeters, Calibrating, Reprints, *Dose equivalents, Californium 252.

A correction is given to published values of the fluence-to-dose-equivalent conversion factor for a

D2O-moderated Cf fission neutron source to account for neutrons between 0.41 eV and 1.0 eV. The corrected value of the conversion factor for all neutrons above 0.41 eV is 10 to the -6th power mrem-sq cm.

501,371

PB85-202125 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Neutron Self-Shielding Factors for Simple Geometries.
Final rept.,
R. F. Fleming. 1982, 6p
Pub. in International Jnl. of Applied Radiation and Isotopes 33, n11 p1263-1268 Nov 83.

Keywords: *Radiation shielding, *Neutrons, Slabs, Spheres, Cylinders, Dosimetry, Reprints, *Self-shielding.

The neutron self-shielding factors are presented for slabs, spheres, and cylinders irradiated in both isotropic and beam neutron fields. Macroscopic cross-sections are tabulated for a number of dosimetry materials for thermal neutrons of 2200 m/s velocity.

18G. Radioactive Wastes and Fission Products

501,372

PB85-183333 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Nuclear Radiation Div.
Uranium-235 Measurement in Waste Material by Resonance Neutron Radiography.
Final rept.,
R. A. Schrack. Nov 84, 7p
Sponsored by Nuclear Regulatory Commission, Washington, DC.
Pub. in Nuclear Technology 67, p326-332 Nov 84.

Keywords: *Radioactive wastes, *Uranium 235, Neutron radiography, Measurement, Reprints.

The use of resonance neutron radiography as a means of monitoring the amount of (235)U in waste material is investigated. A matrix material simulating incinerator ash is inoculated with (235)U in concentrations ranging from 0.00048 to 0.0046 g/cc. The observed uncertainty agrees well with an analytical model and ranges from 16% for the lowest concentration to 2.5% for the highest concentration. The effect of inhomogeneity of matrix and sample is determined and found to be in agreement with analytical models. The technique is demonstrated on sample sizes ranging from 2-l bottles to 55-gal drums.

501,373

PB85-189330 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Office of Nondestructive Evaluation.
Measurements and Standards for Nuclear Waste Management.
Final rept.,
H. T. Yolken. 1980, 1p
Sponsored by American Nuclear Society, LaGrange Park, IL.
Pub. in Proceedings of Annu. Meeting American Nuclear Society, Las Vegas, NV, June 8, 1980, Transactions of the American Nuclear Society 34, 193p.

Keywords: Measurement, Standards, *Radioactive waste management, *Radioactive waste disposal, US NBS.

In August 1979, the Department of Energy (DOE) invited the National Bureau of Standards (NBS) to consider establishment of a technical program that would contribute to the measurement standards foundation required for disposal of nuclear waste. A group of NBS scientists was asked by the management of NBS to examine the needs for measurement standards in nuclear waste management and, if desirable, to recommend a technical program. This talk is an interim report on the progress of their study and states their tentative conclusions and recommendations for an NBS technical program.

501,374

PB85-207363 Not available NTIS

Field 18—NUCLEAR SCIENCE AND TECHNOLOGY

Group 18G—Radioactive Wastes and Fission Products

National Bureau of Standards, Gaithersburg, MD. Polymers Div.

Thermal Expansion of U.S. and Australian Synroc B.

Final rept.,
H. R. Kaese, J. A. Tesk, and E. D. Case. Mar 85, 4p
Pub. in Nuclear Technology 68, p423-426 Mar 85.

Keywords: *Thermal expansion, Radioactive waste processing, Comparison, Reprints, *Radioactive waste disposal, *Synroc process.

For the safe disposal of nuclear waste, a synthetic rock (SYNROC) was developed. Continuing research in this field has led to U.S. and Australian versions of SYNROC B. For both materials, the thermal expansion and expansivity have been determined by the temperature range from 296 to 1100 K.

501,375

PB86-128949

Not available NTIS

National Bureau of Standards (NEL), Gaithersburg, MD. Structures Div.

Reference Laboratory Testing for Backfill.

Final rept.,
R. M. Chung, and F. Y. Yokel. 1982, 9p
Sponsored by Battelle Project Management Div., Columbus, OH. Office of Nuclear Waste Isolation.
Pub. in Proceedings of Annual Meeting of Materials Research Society, Boston, MA., November 1981, Scientific Basis for Nuclear Waste Management, v4 p379-387 1982.

Keywords: *Containers, Compaction, Requirements, Packaging materials, Swelling, Hydraulic conductivity, *Radioactive waste storage, *Backfilling.

Relatively high magnitude of swelling and low hydraulic conductivity are two of the performance requirements for the backfill placed around the radioactive waste package for the underground nuclear waste storage scheme. Some studies have been conducted in U.S. national laboratories and in other countries where the candidate backfill materials were tested under many different conditions to determine the expected range of these properties. This paper briefly examines the variables that were found to be significant in the evaluation of swelling and hydraulic conductivity and special emphasis is placed on the compaction method, compaction effort, and the moisture content at the time of compaction, which do not receive much consideration in ongoing test programs.

501,376

PB86-133428

Not available NTIS

National Bureau of Standards, Gaithersburg, MD. Inorganic Materials Div.

Characterization of Elastic Properties and Microstructure of U.S. and Australian Synroc-B.

Final rept.,
E. D. Case, and T. Negas. 1984, 7p
Sponsored by California Univ., Berkeley. Dept. of Materials Science and Engineering.
Pub. in Adv. Ceram. 8, p723-729 1984.

Keywords: Elastic properties, Microstructure, Australia, Comparison, Reprints, *Synroc process, *Radioactive waste disposal, USA.

The Young's modulus, shear modulus, and Poisson's ratio have been measured for U.S. and Australian versions of Synroc B. Despite some microstructural differences between the U.S. and Australian synroc, their elastic properties are quite similar. For the Australian synroc, thermal anneals in air, at temperatures up to 1285C, resulted in the appearance of numerous voids about 10 micrometers across and some additional voids > 100 micrometers across.

18J. Reactor Materials

501,377

PB85-178051

PC A03/MF A01

National Bureau of Standards (NML), Gaithersburg, MD. Office of Standard Reference Data.

Computerizing Materials Data - A Workshop for the Nuclear Power Industry. The Report of a Workshop Held at Knoxville, Tennessee on May 2-3, 1984.

Final rept.,
J. Rumble, and J. H. Westbrook. Jan 85, 48p NBS/SP-689
Also available from Supt. of Docs as SN003-003-02636-1. Sponsored by Metal Properties Council, Inc., New York, American Society for Metals, Metals Park, OH., American Society for Testing and Materials, Philadelphia, PA., and American Society of Mechanical Engineers, New York. Library of Congress catalog card no. 84-601161.

Keywords: *Materials, Information systems, Networks, Planning, Mechanical properties, Corrosion, Alloys, Ceramics, Polymers, Radiation effects, *Reactor materials, *Nuclear industry, *Data bases, Computer applications, On line systems.

This report summarizes the recommendations of a Workshop in Computerized Materials Data as related to engineers in the Nuclear Power Industry. Four areas of discussion are featured: the content of a proposed data system; its size and data sources; the user interfaces and system capabilities; and ways of making further progress. In addition, changes in the use of materials data in the Nuclear Power Industry and progress-to-date in computerizing these data are presented.

501,378

PB85-196186

Not available NTIS

Development of Uranium Oxide Reference Materials for Gamma-Ray Measurements of the Enrichment.

Final rept.,
R. J. S. Harry, and H. T. Yolken. 1979, 11p
Sponsored by Institute of Nuclear Materials Management, Inc., Piketon, OH.
Pub. in Proceedings of the Institute of Nuclear Material Management Annual Meeting (20th), Albuquerque, NM., July 16-18, 1979, v8 p54-64.

Keywords: *Uranium oxides, Nuclear materials management, Gamma ray spectroscopy, Nondestructive tests, *Reference materials, *Safeguards.

The application of gamma-ray measurements for uranium enrichment determinations is now a mature technique finding widespread use. These facts led the European Safeguards Research and Development Association (ESARDA) Working Group on Techniques and Standards for Non-destructive Analysis to conclude that the development of certified reference materials for low enriched uranium oxide was the next necessary step to enhance the usefulness of the technique. This paper describes the cooperative development of these certified reference materials in the European Community and the United States of America. The following organizations are taking part in the development: The ESARDA working group, the Commission of the European Communities Joint Research Centre - Geel Establishment - Central Bureau for Nuclear Measurements, the U.S. National Bureau of Standards, the New Brunswick Laboratory, and the Los Alamos Scientific Laboratory.

501,379

PB85-201903

Not available NTIS

Tank Volume Calibration Algorithm.

Final rept.,
F. E. Jones. 1984, 12p
Pub. in Nuclear Materials Management 13, n1 p16-27 1984.

Keywords: *Nuclear materials management, *Tanks(Containers), *Volume, *Calibrating, Accountability, Water, Reprints, *Safeguards.

An algorithm has been developed to enable inference of the volume of process mixture in a tank, such as a nuclear materials accountability tank, at temperature T from measurements of differential pressure and temperature and values of other parameters. The differential pressure is converted to that corresponding to water at the reference temperature, 25C, by the use of a derived equation. This differential pressure is then used in a water calibration equation to calculate the volume of water at 25C. This volume is equal to the volume of process mixture at 25C at the same level in the tank, the desired result.

19. ORDNANCE

19D. Explosions, Ballistics, and Armor

501,380

PB85-189249

Not available NTIS

National Bureau of Standards (NEL), Gaithersburg, MD.

Importance of Product Labeling.

Final rept.,
L. K. Eliason. Feb 85, 2p
Sponsored by National Inst. of Justice, Washington, DC.
Pub. in The Police Chief LII, n2 p19-20 Feb 85.

Keywords: Armor, Law enforcement, Marking, Standards, Manufacturers, Litigation, Identifying, Manufacturers, Reprints, *Police equipment, *Product labeling, Product liability.

The article discusses labeling of law enforcement equipment from two aspects: proper identification of the various models of such items, and the role of labeling in product liability on the part of manufacturers and local police departments. Examples of problems resulting from inadequate product labeling are presented, as are cases involving litigation arising from product labeling, with emphasis upon police body armor.

20. PHYSICS

20A. Acoustics

501,381

PB85-170660

Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

Analytical Approach to Acoustic Emission Signal Processing: Problems and Progress.

Final rept.,
N. N. Hsu, and D. G. Eitzen. Oct 84, 9p
Pub. in Proceedings of Int. Acoustic Emission Symposium (7th), Progress in Acoustic Emission 2, Zao, Japan, October 23-26, 1984, p326-334.

Keywords: *Signal processing, Greens function, *Acoustic emissions.

The detected AE voltage waveform is considered as the convolution of (1) the source waveform, (2) the Green's function of the structure and (3) the transduction function of the detector. The authors have demonstrated, both in concept and in controlled experiment, that knowing two of the three functions the remaining unknown function can be determined. However, to solve any of the three the other two must be precisely determined. Many problems remain to be solved. The authors have made some progress in the understanding of these problems. Specifically they will report on the: 1. Design and characterization of simulated transient AE sources. 2. Development of techniques for experimental determination of Green's functions. 3. Development of a new test configuration for AE source characterization for material studies. Finally the authors make some remarks on the comparison of the various approaches to AE waveform analysis.

501,382
PB85-172476 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
New Method of Acoustic Emission Transducer Calibration. Appendix.
Final rept.,
F. R. Breckenridge, and T. Watanabe. Jun 84, 10p
See also AD-A149 837. Sponsored by Army Research Office, Research Triangle Park, NC.
Pub. in Jnl. of Acoustic Emission 3, n2 p59-68 Jun 84.

Keywords: *Transducers, *Calibration, Voltage, Greens function, Frequencies, Emission, Reprints, *Acoustic measurement.

A new method of acoustic emission transducer calibration is developed using numerical solutions of Green's functions in a half space. This method allows transducer calibration without employing elaborate equipment. The calibration curves obtained for six transducers by the present method agree with results obtained by the Nippon Steel Corporation and the National Bureau of Standards.

501,383
PB85-202653 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Correcting for Ray Refraction in Velocity and Attenuation Tomography: A Perturbation Approach.
Final rept.,
S. J. Norton, and M. Linzer. 1982, 33p
Pub. in Ultrason. Imag. 4, n3 p201-233 1982.

Keywords: *Ultrasonic radiation, *Refraction, *Acoustic refraction, Acoustic velocity, Perturbation theory, Correction, Reprints, *Tomography, Acoustic attenuation.

In velocity and attenuation tomography, ray refraction leads to errors in time-of-arrival, as well as to errors in attenuation due to phase cancellation and lateral beam displacement. Some authors have proposed iterative techniques based on ray tracing to correct for these effects. In this paper, the authors consider an alternative approach using a perturbation analysis of refraction. This approach requires neither iteration nor ray tracing. In both two and three dimensions, the perturbation approach is much simpler computationally than ray tracing methods. Computer simulated reconstructions are presented which clearly show the improvement that can be achieved with the second-order time delay correction.

501,384
PB85-202901 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Thermophysics Div.
Scattering of Sound Waves by Inhomogeneities: Time Domain Analysis.
Final rept.,
R. D. Mountain, and G. Birnbaum. 1984, 7p
Pub. in Nondestructive Testing Communications 1, p219-225 1984.

Keywords: *Acoustic scattering, *Nondestructive tests, Acoustic measurement, Ultrasonic tests, Solids, Reprints, Born approximation.

The scattering of sound waves by isolated inhomogeneities in an otherwise uniform solid is analyzed using the Born approximation in the time domain. The volume and shape of the scatterer is related to time moments of the amplitude of the scattered signal. The matching of the incident pulse shape to the size of the scatterer is found to be essential if this type of measurement is to yield useful results.

501,385
PB86-119252 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD.
Acoustical Research in the Physical Sciences - Properties of Gases, Liquids, and Solids.
Final rept.,
M. Greenspan. 1980, 7p
Pub. in Jnl. of Acoustical Society of America 68, n1 p29-35 1980.

Keywords: *Acoustics, Ultrasonic radiation, Acoustic absorption, Reprints, Dispersion.

In June, 1979 the Acoustical Society of America celebrated its 50th anniversary at its 97th meeting in Cambridge, Mass. As a special feature there was held each day a plenary session, attended by about 1000 people,

at which the history, from 1929 until the present, of the several branches of acoustics was treated by about a dozen speakers. The present author was chosen to speak for one-half hour on physical acoustics as it relates to other branches of physics. The paper is a nearly verbatim rendering of this talk. It is intended to be intelligible to the non-specialist and has only one equation. The major emphasis is on relaxation phenomena in fluids.

501,386
PB86-124104 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Traceability of Acoustical Instrument Calibration to the National Bureau of Standards.
Final rept.,
V. Nedzelnitsky. 1980, 4p

Pub. in Proceedings of International Conference on Noise Control Eng. Noise Control for the 80's, Miami, FL., December 8-10, 1980, Inter-Noise 80, v2 p1043-1046.

Keywords: *Acoustic measurement, *Calibrating, *Microphones, Electroacoustic transducers, Metrology.

The necessity for the National Bureau of Standards (NBS) to provide absolute, reciprocity-based pressure and free-field calibrations of measuring microphones sufficiently accurate for the most critical needs creates a hierarchy of instrument calibration establishing direct or implied chains of 'traceability' to the NBS. Different users have differing needs so that 'traceability' is not the same concept for all users. In analyzing various definitions of traceability, Belanger ('Traceability: An Evolving Concept,' ASTM Standardization News, Jan. 1980, pp. 22-27) described two contrasting views. Each of these views is shown in the present paper to represent the primary concern of a group of users of the NBS acoustic calibration services. Whichever view is employed, the value of a given system for realizing traceability depends on that system's capacity to ensure measurements of adequate accuracy.

20B. Crystallography

501,387
PB85-183325 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.
Transport in a Disordered One-Dimensional System: A Fractal View.
Final rept.,
R. J. Rubin. Sep 84, 10p
Pub. in Jnl. of Statistical Physics 36, n5/6 p615-624 Sep 84.

Keywords: *Crystal defects, Transport properties, Reprints, One dimensional, Fractals.

The author reexamines the calculation of the transmission coefficient of a random array of N isotopic defects in an otherwise perfect, harmonic, one-dimensional crystal lattice. The thermal conductivity of this model system has been studied under steady-state conditions in which there is a kinetic temperature difference across, and an associated energy flux through, the array of defects. An exact expression for the transmission coefficient is obtained in terms of the magnitude of an N th order determinant. Rubin reduced the evaluation of the determinant to the evaluation of a sequence of N-1 nonlinear transformations drawn from a set of transformations parametrized by the nearest-neighbor spacing of the isotopic defects. These transformations are self-inverse and provide an example of what Mandelbrot has termed a self-inverse fractal. The variety of limiting distributions of values obtained under these transformations will be illustrated.

501,388
PB85-184554 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Comparison of Methods for Reducing Preferred Orientation.
Final rept.,
L. D. Calvert, A. F. Sirianni, G. J. Gainsford, and C. R. Hubbard. 1982, 6p
Sponsored by Denver Research Inst., CO.
Pub. in Chapter in Advances in X-Ray Analysis, v26 p105-110 1982.

Keywords: *Molybdenum oxides, *Phlogopite, *Mica, Orientation, X ray diffraction, Comparison, Reprints, *Fluorophlogopites.

Spray drying and liquid phase spherical agglomeration methods to orientation free prepare spherical agglomerates were tested for MoO₃ and fluorophlogopite mica. Reflection geometry with CuK(alpha) radiation, Debye-Scherrer geometry with MoK(alpha) radiation and theoretical calculations are compared. Both methods of preparation of spherical agglomerates gave excellent results with the Debye-Scherrer geometry. Spray dried spheres gave good agreement for reflection geometry. Only spray dried spheres could be used with reflection geometry.

501,389
PB85-184802 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Oscillatory Morphological Instabilities Due to Non-Equilibrium Segregation.
Final rept.,
S. R. Coriell, and R. F. Sekerka. 1983, 10p

Pub. in Jnl. of Crystal Growth 61, n3 p499-508 1983.

Keywords: *Crystal growth, *Solidification, Perturbation theory, Alloys, Reprints, Instability.

Linear perturbation theory is used to study morphological instability for rapid directional solidification at constant velocity under conditions where there is significant departure from local equilibrium at an initially planar solid-liquid interface. When present, oscillatory instabilities lead to a three dimensional segregation pattern in which periodic solute variations in the two transverse directions are modulated by a periodic variation in the direction of growth.

501,390
PB85-189215 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.
Epitaxial Crystal Growth in Gadolinium on Tungsten.
Final rept.,
A. Ciszewski, and A. J. Melmed. 1984, 4p
Pub. in Surface Science 145, pL471-474 1984.

Keywords: *Gadolinium, *Diffusion, *Surfaces, Tungsten, Epitaxy, Substrates, Crystal growth, Reprints, Field ion microscopy.

Field electron microscopy is used to measure activation energies for multilayer diffusion of gadolinium over several different surfaces of tungsten and to prepare crystal layers of gadolinium by epitaxy on tungsten substrates. Nucleation, crystal growth, and epitaxial relations are described.

501,391
PB85-189223 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.
'Surface Self-Diffusion of Dysprosium and Gadolinium'.
Final rept.,
A. Ciszewski, and A. J. Melmed. 1984, 4p
Pub. in Surface Science 145, pL509-L512 1984.

Keywords: *Dysprosium, *Gadolinium, *Diffusion, *Surfaces, Epitaxy, Substrates, Tungsten, Reprints, *Self diffusion, Field electron microscopy.

Measurements of activation energy for surface self-diffusion are reported for dysprosium and gadolinium. The specimens were prepared by epitaxial crystal growth on clean tungsten substrates in an ultrahigh vacuum field electron microscope. Results are compared to earlier data for other metals.

501,392
PB85-196004 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.

Field 20—PHYSICS

Group 20B—Crystallography

Advanced Multi-Chamber System for Preparation of Amorphous Thin Films by Coevaporation and Their Subsequent Characterization by AES (Auger Electron Spectroscopy), ESCA (Electron Spectroscopy for Chemical Analysis), SIMS (Secondary Ion Mass Spectroscopy), and ISS (Ion Scattering Spectroscopy) Methods.

Final rept.,
D. M. Sanders, E. N. Farabaugh, W. S. Hurst, and W. K. Haller. 1981, 3p
Pub. in Jnl. of Vacuum Science and Technology 18, n3 p1308-1310 Apr 81.

Keywords: *Thin films, Electron beams, Silicon dioxide, Magnesium oxides, Preparation, Reprints, *Amorphous materials, *Coevaporation.

Vacuum deposition is one means of producing amorphous structures from compositions which do not normally form glasses. Aluminum oxide, for instance, is always polycrystalline when solidified from the melt, but frequently has highly disordered structures when produced by vacuum evaporation. Preparation of complex multicomponent thin films by single source vacuum evaporation is normally limited by the large differences in vapor pressures of the components. One approach which overcomes this difficulty involves co-deposition from multiple sources operated at appropriate temperatures to produce the desired individual deposition rates. In this paper, the authors describe a facility which has been designed and constructed for the production of thin films by multiple source evaporation and subsequent analysis by Auger Electron Spectroscopy (AES), Electron Spectroscopy for Chemical Analysis (ESCA), Secondary Ion Mass Spectroscopy (SIMS) and Ion Scattering Spectroscopy (ISS). The authors then present initial results obtained on the system MgO-SiO₂ showing the functional relationship between the concentration of the second component (in this case SiO₂) and the crystallinity of the film.

501,393

PB85-196020 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Use of the Pearson Type VII Distribution in the Neutron Profile Refinement of the Structures of LiReO₃ and Li₂ReO₃.

Final rept.,
A. Santoro, R. J. Cava, D. W. Murphy, and R. S. Roth. 1982, 4p
Sponsored by Argonne National Lab., IL., and Argonne Universities Association, IL.
Pub. in AIP Conference Proceedings of Symposium on Neutron Scattering, Argonne, IL., August 12-14, 1981, n89 p162-165 1982.

Keywords: *Crystal structure, Neutron diffraction, *Lithium renates.

The crystal structures of the compounds LiReO₃ and Li₂ReO₃ have been refined with the Rietveld method. Neutron powder diffraction data collected at room temperature were used in these calculations. Since the shapes of the diffraction lines for both materials could not be approximated by Gaussians with sufficient accuracy, the Pearson type VII function was used in all refinements. The value of *m* was assumed to be 2 theta-independent in these calculations. The best fits to the experimental observations were obtained with *m* = 1.5 for LiReO₃ and *m* = 3 for Li₂ReO₃. Both compounds crystallize with the symmetry of space group R3c, and the lattice parameters (hexagonal axes) are *a* = 5.0918(3), *c* = 13.403(1) Å for LiReO₃ and *a* = 4.9711(4), *c* = 14.788(1) Å for Li₂ReO₃.

501,394

PB85-201929 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Reply to 'Comment on 'On the Atomic Structure of (001) Tungsten'.

Final rept.,
A. J. Melmed, and W. R. Graham. 1982, 3p
Pub. in Surface Science 123, n1 pL706-L708 1982.

Keywords: *Tungsten, *Atomic structure, *Surfaces, Phase transformations, Reprints, Field ion microscopy, Low energy electron diffraction.

A reply to comment by P. J. Estrup, L. D. Roelofs, and S. C. Ying is given.

501,395

PB85-202000 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.

Powder-Pattern: A System of Programs for Processing and Interpreting Powder Diffraction Data.

Final rept.,
N. P. Pyrras, and C. R. Hubbard. 1983, 10p
Sponsored by JCPDS-International Centre for Diffraction Data, Swarthmore, PA.
Pub. in Advances in X-Ray Analysis 26, p63-72 1983.

Keywords: *X ray diffraction, *Crystal structure, Data processing, Spectrum analysis, Fortran, Reprints, *Powder patterns, POWDER-PATTERN system, Computer applications.

POWDER-PATTERN is a general system for processing powder diffraction data. The system has been designed and developed specifically for the processing of high quality standard x-ray diffraction powder patterns. POWDER-PATTERN is an interactive system that consists of a number of independent modules (programs) that have been designed so that they allow recycling in the execution of the modules. The modules are linked through the use of a common file named PKS that serves as an input to the modules and as a depository of the data generated by the different modules and by the user. An editing program allows for the manipulation of the PKS file. Modules locate the peaks, refine the parameters with profile refinement, correct the observed peak positions for external and internal calibration, and perform a least squares cell refinement. Interactive plotting programs allow the user to intervene at various stages of the processing, or to simply check the results. The profile refinement module using flexible rational profiles with a relatively small number of parameters can give accurate peak positions and can help in the interpretation of complicated bands with overlapping profiles.

501,396

PB85-205862 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Structure of LaTaO₄ at 300C by Neutron Powder Profile Analysis.

Final rept.,
R. J. Cava, and R. S. Roth. 1981, 9p
Pub. in Jnl. of Solid State Chemistry 36, n2 p139-147 1981.

Keywords: *Crystal structure, Neutron diffraction, Reprints, *Lanthanum tantalates.

LaTaO₄ above 175C is orthorhombic, space group A2(1)am, with *a* = 5.6643(1), *b* = 14.6411(3), *c* = 3.9457(1), and *z* = 4(1). Orthorhombic LaTaO₄ is isostructural with the room temperature BaMnF₄. Orthorhombic CeTaO₄ and PrTaO₄ are isostructural.

501,397

PB85-222115 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Symmetry in Solid State Transformation Morphologies.

Final rept.,
J. W. Cahn, and G. Kalonji. 1982, 12p
Sponsored by Carnegie-Mellon Univ., Pittsburgh, PA, American Society for Metals, Metals Park, OH, and National Science Foundation, Washington, DC.
Pub. in Proceedings of Int. Conf. Solid to Solid Phase Transformations, Pittsburgh, PA., August 10-14, 1981, p3-14 1982.

Keywords: *Bicrystals, Crystal symmetry, Phase transformations, Interfaces, Crystal morphology.

Crystallographic symmetry is an important factor in determining the morphologies of crystals grown from (or embedded in) crystalline matrices. The rules for obtaining the appropriate bicrystal morphologies (forms and variants) from symmetries of the individual crystals and their relative orientation are examined and applied to specific examples. The role of symmetry dictated extrema in specifying orientation relationships resulting from certain physical processes such as homogeneous nucleation, is discussed.

501,398

PB85-222255 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Structural Aspects of Lithium Insertion in Oxides: Li_xReO₃ and Li₂FeV₃O₈.

Final rept.,
R. J. Cava, A. Santoro, D. W. Murphy, S. Zahurak, and R. S. Roth. Oct 81, 4p
Sponsored by Oak Ridge National Lab., TN, General Electric Co., Washington, DC, National Science Foundation, Washington, DC, and Office of Naval Research, Arlington, VA.

Pub. in Proceedings of Int. Conf. Fast Ionic Transport in Solids, Gatlinburg, TN., May 18-22, 1981, Solid State Ionics 5, p323-326 Oct 81.

Keywords: *Crystal structure, Neutron diffraction, *Lithium renates, *Lithium iron vanadates.

The authors have determined the crystal structures of LiReO₃, Li₂ReO₃ and Li₂FeV₃O₈, obtained by Li insertion of ReO₃ and FeV₃O₈, by neutron diffraction powder profile analysis. The ReO₃ host lattice is exclusively corner shared and undergoes significant twisting on Li insertion. The FeV₃O₈ host lattice is extensively edge shared and changes little on Li insertion. The Li is accommodated in 6 coordinate sites in the renates and 5 coordinate sites in the iron vanadate.

501,399

PB85-229300 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.

Effect of Anisotropic Crystal-Melt Surface Tension on Grain Boundary Groove Morphology.

Final rept.,
P. W. Voorhees, S. R. Coriell, G. B. McFadden, and R. F. Sekerka. 1984, 17p
Pub. in Jnl. of Crystal Growth 67, n3 p425-440 Aug 84.

Keywords: *Interfacial tension, *Grain boundaries, Crystal growth, Interfaces, Anisotropy, Reprints.

The shape of a stationary solid-liquid interface in a temperature gradient near a grain boundary in a pure material is calculated for anisotropic crystal-melt surface tension and equal thermal conductivities of crystal and melt. Results are compared with those for the well-known problem of the two-dimensional equilibrium shape of a crystal. For small anisotropy, the resulting interface shapes have continuously turning tangents but differ in detail from the grain boundary groove shapes that have been calculated for isotropic surface tension. For larger anisotropy, the interface shapes have discontinuities in slope as a result of missing orientations; these missing orientations are the same as those that would be missing on the corresponding equilibrium interface shape. In cases where a normal to the grain boundary or to the macroscopic interface is in the range of missing orientations on the corresponding equilibrium shape, the groove shape may contain some of these orientations as well as having varifold surfaces. Detailed numerical results are presented for a surface tension with fourfold symmetry.

501,400

PB85-229359 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Semiconductor Materials and Processes Div.

In situ Alignment Procedure for X-ray Topography.

Final rept.,
R. A. Forman, and S. Mayo. 1985, 5p
Pub. in Jnl. of Applied Crystallography 18, p106-109 1985.

Keywords: *Alignment, X ray diffraction, Gallium arsenides, Silicon, Reprints, *X ray topography, Semiconductors.

A simple method for in situ alignment of samples in a double crystal x-ray topography system is described. The method permits a specific crystallographic axis to be made coincident with the sample rotation axis used to set the Bragg angle. Surface reflections from approximately orthogonal crystallographic planes are required, and tables of such planes suitable for alignment of cubic crystals are given. The procedure allows rapid setup for the other accessible surface reflection or transmission topographies.

501,401

PB85-229979 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Inorganic Materials Div.

Phase Transition and Compression of LiNbO₃ Under Static High Pressure.

Final rept.,
J. A. H. da Jornada, S. Block, F. A. Mauer, and G. J. Piermarini. 1985, 4p
Sponsored by Conselho Nacional de Pesquisas, Rio de Janeiro (Brazil), and Universidade Federal do Rio Grande do Sul, Porto Alegre (Brazil). Inst. de Fisica.
Pub. in Jnl. of Applied Physics 57, n3 p842-844, 1 Feb 85.

Keywords: *Lattice parameters, X ray diffraction, Phase transformations, Compressive properties, Reprints, *Lithium niobates, High pressure, Pressure dependence, Cubic lattices.

Lattice parameters of LiNbO₃ were measured at room temperature over the pressure range 0-35 GPa by x-ray diffraction using the diamond anvil cell. In the region below 13 GPa (where a hydrostatic pressure was maintained) the pressure dependence of the volume can be well described by the Birch-Murnaghan equation of state, yielding $B(0) = 134 \pm 3$ GPa for the zero-pressure bulk modulus and $B'(0) = 2.9 \pm 0.5$ for its pressure derivative. A phase transformation was detected at 30 ± 3 GPa both by x-ray diffraction and by optical observation of the change from a transparent to an opaque state. The pattern of the high-pressure phase was tentatively indexed on the basis of a cubic cell with $a = 6.78$ Å.

501,402
PB86-103611 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.
Epitaxial Crystal Growth of hcp Metals on bcc Metals: Dysprosium on Tungsten.
Final rept.,
A. Ciszewski, and A. J. Melmed. 1984, 7p
Pub. in Jnl. of Crystal Growth 69, p253-259 1984.

Keywords: *Dysprosium, *Tungsten, *Epitaxy, *Crystal growth, Body centered cubic lattices, Hexagonal close packed lattices, Surfaces, Diffusion, Nucleation, Reprints, Field emission microscopy.

Surface diffusion of dysprosium on tungsten is discussed and activation energies for multilayer diffusion over various substrate planes are measured. Nucleation and epitaxial crystal growth are investigated and it is shown that single crystal or polycrystal layers can be grown under controlled conditions in the field emission microscope. The epitaxial relationships are given.

501,403
PB86-105822 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.
Analysis of Angular Dependent XPS (X-ray Photoelectron) Peak Intensities.
Final rept.,
R. A. Armstrong, and W. F. Egelhoff. 1985, 8p
Pub. in Surface Science 154, pL225-L232 1985.

Keywords: *Epitaxy, Nickel, Copper, Cobalt, Metal films, Substrates, Surfaces, Reprints, *X-ray photoelectron spectroscopy.

Angle resolved X-ray photoelectron (XPS) studies of clean Ni(100) and of epitaxial Cu and Co films on Ni(100) have been interpreted with the aid of single scattering cluster calculations. It is found that for atoms in the top few atomic layers, photoelectron forward scattering by overlying atoms in the lattice causes XPS peak intensities to be enhanced at angles corresponding to nearest neighbor and next-nearest neighbor internuclear axes. Angle resolved XPS should thus be an excellent approach for gaining structural information on, for example, epitaxial overlayers or surface reconstructions.

501,404
PB86-114030 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Raman and X-ray Investigations of Ice VII.
Final rept.,
F. A. Mauer, S. Block, G. J. Piermarini, and R. Munro. 1982, 3p
See also AD-A116 900.
Pub. in AIRAPT Conference on High Pressure in Research and Industry (8th), Uppsala, Sweden, August 17-22, 1981, Assoc. Int. pour l'Avancement de la Recherche et de la Technologie aux Hautes Pressions 2, p537-539 1982.

Keywords: *Ice, *Crystal structure, Raman spectroscopy, X ray diffraction, High pressure.

Ice VII has been studied in a diamond anvil cell at room temperature by Raman spectroscopy to 30.0 GPa and energy dispersive x-ray diffraction to 36.0 GPa. Both the O-O distance and the Raman O-H frequency decrease with pressure and they are linear relative to each other within experimental error. The decrease in the Raman frequency is related to the increase in length of the O-H bond towards a symmetrical O...H...O hydrogen bond. Generally the lattice parameter at

each pressure is based on the (110), (200), and (211) reflections. The largest portion of the error is due to the uncertainty of the pressure in the highest ranges arising from the nonhydrostatic character. The pressure range measured by the ruby fluorescence method in a sample approximately 0.2 mm in diameter by 0.1 mm thick ranged from 23.7 GPa to 26.2 GPa. In addition to the ice results, the advantages of the double-slit energy dispersive x-ray diffraction system is briefly described.

501,405
PB86-115664 PC A07/MF A01
National Bureau of Standards (NML), Gaithersburg, MD.
Standard X-ray Diffraction Powder Patterns: Section 21 - Data for 92 Substances.
Final rept.,
M. C. Morris, H. F. McMurdie, E. H. Evans, B. Paretkin, and H. S. Parker. Sep 85, 146p NBS-MONO-25-SECT-21
See also PB84-155191. Also available from Supt. of Docs as SN003-003-02690-5. Prepared in cooperation with JCPDS-International Centre for Diffraction Data, Swarthmore, PA.

Keywords: *Crystal structure, *X ray diffraction, *Standards, Lattice parameters, Inorganic compounds, Tables(Data), *Powder patterns.

Standard x-ray powder diffraction patterns are presented for 92 substances. These patterns, useful for identification, were obtained by automated diffractometer methods. The lattice constants from the experimental work were refined by least-squares methods, and reflections were assigned hkl indices consistent with space group extinctions. Relative intensities, calculated densities, literature references, and other relevant data are included.

501,406
PB86-119286 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Quantum Metrology Group.
Two-Dimensional X-ray Scattering.
Final rept.,
S. Brennan. 1985, 9p
Sponsored by Department of Energy, Washington, DC., National Science Foundation, Washington, DC., and National Institutes of Health, Bethesda, MD.
Pub. in Surface Science 152/153, p1-9 1985.

Keywords: *Surfaces, X ray diffraction, Metal films, Lead(Metal), Copper, Epitaxy, Substrates, Reprints, *X ray scattering, *Grazing incidence scattering, Two dimensional.

A discussion of Grazing Incidence Scattering (GIS) is presented, with an emphasis on applications of the technique. This paper is an overview of what can and has been done in this new area of surface structural science. The method is contrasted to some of the currently available techniques to show why it offers unique advantages for certain classes of problems such as the crystallography of ordered overlayers, clean reconstructed surfaces and the thermodynamics of two-dimensional melting. Some recent data for Pb layers on Cu(110) are presented to indicate the type of information that this new method can obtain. Also discussed is the application of the technique to the interfacial structure of epitaxial layers focusing on in-plane strain, lattice mismatch and the abruptness of the substrate-epitaxial interface.

501,407
PB86-129079 Not available NTIS
National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.
Displacement Field of a Dislocation Distribution.
Final rept.,
R. de Wit. 1981, 6p
Pub. in Proceedings of International Conference on Dislocation Modelling of Physical Systems, Gainesville, FL., June 22-27, 1980, p304-309 1981.

Keywords: Elastic properties, Anisotropy, Displacement, *Dislocations, Burgers vector.

Burgers' formula gives the displacement field due to a discrete dislocation line of arbitrary shape in an isotropic, linearly-elastic, infinitely extended, homogeneous body. The paper derives the analogous expression for a continuous distribution of dislocations in an anisotropic body. Special cases give the displacement due to a discrete dislocation line in anisotropic elasticity and due to a continuous dislocation distribution in iso-

tropic elasticity. These expressions all represent generalization of Burgers' original formula.

501,408
PB86-129590 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Thermophysics Div.
Relative Stability of Dense Crystalline Packings.
Final rept.,
H. J. Raveche, and R. D. Mountain. 1985, 3p
Pub. in Physical Review B: Condensed Matter 31, n11 p7446-7448, 1 Jun 85.

Keywords: *Crystal structure, Hexagonal lattices, Free energy, Stability, Reprints.

Close-packed crystalline arrangements of spherical particles interacting via the inverse-twelfth-power intermolecular potential are studied by molecular-dynamics simulations. For systems of 576 and 4608 particles under the condition of constant total energy, the different structures exhibit the same pressure and temperature at high densities, within the accuracy of the computations. The consequences of this apparent degeneracy in determining the relative stability of stackings of hexagonally packed layers are discussed.

501,409
PB86-129632 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Reactor Radiation Div.
Dynamics of Dilute H in Beta-Phase Palladium Deuteride: A Novel Mass Defect.
Final rept.,
J. J. Rush, J. M. Rowe, and D. Richter. 1985, 2p
Pub. in Physical Review B: Condensed Matter 31, n9 p6102-6103, 1 May 85.

Keywords: *Crystal defects, Deuterium compounds, Lattice vibrations, Reprints, *Palladium hydrides.

The authors present a neutron scattering study of the vibrations of a light-atom defect which, in contrast with earlier studies, is both chemically identical to and half the mass of its heavy-atom host, namely, 3.7 at % H in beta-palladium deuteride. They observe a large shift in hydrogen vibration modes from those in beta-PdH, which is in close agreement with the local-mode frequency predicted for an isolated mass defect and provides a prototype example for such a system.

501,410
PB86-129764 Not available NTIS
National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.
Dislocation Concepts Applied to Material Modeling.
Final rept.,
R. de Wit. 1985, 16p
Sponsored by American Society for Metals, Metals Park, OH., and Army Research Office, Arlington, VA.
Pub. in Proceedings of International Symposium on Mechanics of Dislocation, Houghton, ML., August 28-30, 1983, p111-126 1985.

Keywords: Plastic deformation, Microstructure, Work hardening, Homotropy theory, Differential geometry, Liquid crystals, Reviews, *Dislocations, Amorphous materials.

A selective survey is given of several research areas where dislocation concepts have made useful contributions to our understanding of the physical world. The value of dislocation theory for interpreting plastic deformation and work hardening is discussed. Dislocation concepts have led to elegant continuum theories which are closely related to differential geometry and have analogies in electrodynamics and relativity. Dislocation concepts are also useful in fields other than solid crystals, surface crystals, liquid crystals, magnetism, amorphous materials, and waves. Finally, some speculations are given for the application of dislocations in solid state technology.

501,411
PB86-133535 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Reactor Radiation Div.
Structure of ND₄NO₃ Phase-V by Neutron Powder Diffraction.
Final rept.,
C. S. Choi, and H. J. Prask. 1983, 7p
Pub. in Acta Crystallographica Section B-Structural Science 39, p414-420 1983.

Field 20—PHYSICS

Group 20B—Crystallography

Keywords: *Ammonium nitrate, *Crystal structure, Deuterium compounds, Neutron diffraction, Phase transformations, Twinning, Thermal expansion, Reprints.

The crystal structure of ND₄NO₃ phase V was determined by the Rietveld refinement method for a series of neutron powder diffraction data measured at temperatures ranging from 10K to 250K using a 90% deuterated sample. The structure was found to be orthorhombic Pccn, $a = 7.8850(2)$, $b = 7.9202(2)$, $c = 9.7953(2)$, and $Z = 8$. The final R-indices were $R(\text{int}) = .036$, $R(\text{prof}) = .024$ for the 78K structure. The cations and anions are packed with a distorted CsCl-type arrangement and are linked together by two sets of three-dimensional hydrogen bond chains. There are no other polymorphic phases (i.e. phase VII) down to 10K. The thermal expansions of phases V, IV, III, and II were also measured in the study.

501,412
PB86-133576 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Quantum Metrology Group.
Diffraction of Evanescent X-rays: Results from a Dynamical Theory.
Final rept.,
P. L. Cowan. 1985, 3p
Pub. in Physical Review B: Condensed Matter 32, n8 p5437-5439, 15 Oct 85.

Keywords: *X ray diffraction, Surfaces, Interfaces, Crystal structure, Reprints.

Evanescent x rays can be made to diffract from periodic structures parallel to a surface or interface. A dynamical theory of diffraction yields several novel predictions which may be experimentally important. First, x-ray standing-wave fields are generated and can be controlled. This suggests a new technique for unambiguous determination of surface structure. Secondly, evanescent x-ray wave fields may be produced in the incident medium as well as the substrate. Finally, the rocking curve of the diffracted beam is narrow and asymmetric.

501,413
PB86-136785 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Metallurgy Div.
Observation of Dislocation Images in Surface Reflection by Synchrotron Radiation Topography.
Final rept.,
R. C. Dobbyn, and K. C. Yoo. 1984, 10p
Pub. in Applied X-ray Topography Methods Mater. Sci., p241-250 1984.

Keywords: *Diffraction, Single crystals, Copper, Zinc, Synchrotron radiation, X rays, Surfaces, Reflection, Reprints, *Dislocations.

Dislocation images from copper and zinc single crystals have been obtained by monochromatic synchrotron topography for the purpose of documenting the changes in diffraction contrast as a function of deviations of the incident radiation from the exact Bragg condition and deviations in the observation directions about the Bragg angle. The observed diffraction contrast changes are analyzed and compared with the predictions of the dynamical theory for diffraction in real (imperfect) crystals. Observations were made in real time and recorded on video tape and film at the Cornell High Energy Synchrotron Source (CHESS).

501,414
PB86-136918 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.
X-ray Photoelectron and Auger-Electron Forward Scattering: A New Tool for Studying Epitaxial Growth and Core-Level Binding-Energy Shifts.
Final rept.,
W. F. Egelhoff. 1984, 4p
Pub. in Physical Review B 30, n2 p1052-1055, 15 Jul 84.

Keywords: Copper, Nickel, Surfaces, Reprints, *Auger electron spectroscopy, *X ray photoelectron spectroscopy, *Epitaxial growth, Binding energy.

Above a few hundred eV kinetic energy, Auger electrons and photoelectrons exhibit strong forward scattering by overlying atoms, and this produces intensity peaks at polar and azimuthal angles corresponding to internuclear axes. This provides a new structural probe which is especially useful for studying epitaxy, surface

alloying, and surface segregation. It also provides a new approach to measuring core-level binding-energy shifts by permitting selective enhancement of bulk versus surface signals.

501,415
PB86-136926 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.
New Tool for Studying Epitaxy and Interfaces: The XPS (X-ray Photoelectron Spectroscopy) Searchlight Effect.
Final rept.,
W. F. Egelhoff. 1985, 3p
Pub. in Jnl. of Vacuum Science and Technology A3, n3 p1511-1513 May/Jun 85.

Keywords: Copper, Nickel, Substrates, Interfaces, Reprints, *X ray photoelectron spectroscopy, Epitaxial growth.

Very recently, a phenomenon long known in angle-resolved 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 this 'XPS searchlight' effect as a new tool for studying epitaxy and interfaces.

501,416
PB86-136934 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.
Growth Morphology Determination in the Initial Stages of Epitaxy by XPS (X-ray Photoelectron Spectroscopy).
Final rept.,
W. F. Egelhoff. 1984, 3p
Pub. in Jnl. of Vacuum Science and Technology A-Vacuum Surfaces and Films 2, n2 p350-353 1984.

Keywords: *Copper, Nickel, Substrates, Reprints, *Epitaxial growth, *X ray photoelectron spectroscopy, *Auger electron spectroscopy.

It is found that for Cu(100) and Ni(100) x-ray photoelectrons and Auger electrons with energies of about 1000 eV exhibit intensity variations versus polar angle which are dominated by forward scattering off neighboring atoms. In monitoring the epitaxial growth of Cu on Ni(100) this phenomenon is shown to yield clear and easily available structural information about the arrangement of atoms in the Cu adlayers.

501,417
PB86-138062 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.
Measurement of Time-Dependent Sputter-Induced Silver Segregation at the Surface of a Ni-Ag Ion Beam Mixed Solid.
Final rept.,
J. Fine, T. D. Andreadis, and F. Davarya. 1983, 10p
Pub. in Proceedings of International Conference on Ion Beam Modification of Materials (3rd), Grenoble, France, September 6-10, 1982, Nuclear Instruments and Methods in Physics Research, v209-210, pt 1 p521-530 1983.

Keywords: Ion beams, Diffusion, Separation, Nickel, Silver, Interfaces, Surfaces, *Ion bombardment, *Physical radiation effects, Argon ions.

Sputter depth profiling of alloys and interfaces using low energy ion beams can cause in-depth compositional changes to occur. One possible mechanism responsible for such changes is enhanced diffusion occurring along point defects generated by the ion bombardment in the near surface region. Sputter profiling of a Ni/Ag interface produces a mixed Ni-Ag surface region and the authors have found that in such a region, bombarded with 1 to 4 keV argon ions at 20C, that the Ag will segregate to the surface. The segregation can be observed to occur in real time after the ion bombardment has been stopped. Auger spectroscopy was used to obtain a unique set of measurements of the kinetics of surface segregation due to bombardment enhanced near-surface diffusion. The kinetics of the segregation is examined and its influence on sputter depth profiling demonstrated.

501,418
PB86-140241 Not available NTIS

National Bureau of Standards, Gaithersburg, MD.
Microscopic Evidence for Quasi-Periodicity in a Solid with Long-Range Icosahedral Order.
Final rept.,
D. Shechtman, D. Gratias, and J. W. Cahn. 1985, 6p
Pub. in C. R. Acad. Sc. Paris 11, n18 p909-914, 14 May 85.

Keywords: *Aluminum manganese alloys, *Crystal structure, Electron microscopy, Twinning, Reprints, Penrose tiling.

The authors demonstrate with high resolution electron microscopy that the icosahedral phase in aluminum manganese alloys has many of the topological features of a three-dimensional Penrose tiling. They rule out twinning and conventional modulated structures as alternate explanations for the structure, and suggest a classification scheme based on hyperspace crystallography.

501,419
PB86-165933 (Order as PB86-165776, PC A08/MF A01)
National Institutes of Health, Bethesda, MD.
Fourier Representations of Pdf's Arising in Crystallography.
G. H. Weiss, and U. Shmueli. 24 Jun 85, 9p
Prepared in cooperation with Tel-Aviv Univ. (Israel). Sponsored by National Bureau of Standards, Gaithersburg, MD.
Included in Jnl. of Research of the National Bureau of Standards, v90 n6 p507-515 Nov-Dec 85.

Keywords: *Crystallography, *Fourier series, *Probability density functions, Crystal structure, Central limit theorem.

A survey is given of some recent calculations of univariate and multivariate probability density functions (pdf's) of structure factors used to interpret crystallographic data. The authors have found that in the presence of sufficient atomic heterogeneity the frequently used approximations derived from the central limit theorem in the form of Edgeworth or Gram-Charlier series can be quite unreliable, and in these cases the more exact, but lengthier, Fourier calculations must be made.

501,420
PB86-166774 PC A05/MF A01
National Bureau of Standards, Gaithersburg, MD. Reactor Radiation Div.
NBS*LATTICE - A Program to Analyze Lattice Relationships. Version of Summer, 1985.
Final rept.,
V. L. Himes, and A. D. Mighell. Dec 85, 84p NBS/TN-1214
Also available from Supt. of Docs as SN003-003-02713-8.

Keywords: *Crystal structure, *Crystal lattices, Computer programming, Crystal symmetry, Fortran, NBS star LATTICE computer program, Matrix inversion.

A FORTRAN program to analyze lattice relationships has been written and is available for distribution by the NBS Crystal Data Center. The present version of NBS *LATTICE performs several functions including: (1) the characterization and identification of unknown materials using lattice-formula matching techniques; (2) the calculation of the reduced cell of the lattice, and the calculation and reduction of specified derivative supercells and/or subcells (i.e., this program function calculates the standard cells which are useful in the determination of metric lattice symmetry, in finding a matrix relating two unit cells, etc.); (3) unit cell transformations; and (4) matrix inversions. It is planned to incorporate additional functions in forthcoming versions of this program. Among others, these functions will include a matrix method to determine metric lattice symmetry and a technique to find a transformation matrix relating any two unit cells.

20C. Electricity and Magnetism

501,421
PB85-183564 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.

Correction to the Formula for the London Moment of a Rotating Superconductor.

Final rept.,
R. M. Brady. 1982, 18p
Sponsored by Trinity Coll., Cambridge (England), and Science Research Council, London (England).
Pub. in Jnl. of Low Temperature Physics 49, n1-2 p1-17 1982.

Keywords: *Superconductors, *Rotation, Magnetic fields, Reprints, London equation, Order parameters, Quantum mechanics.

This paper gives full quantum-mechanical analysis of the magnetic field (first discussed by London) which appears spontaneously when a sample of superconductor is set into rotation. It shows that, for slow rotation velocities and using certain approximations, the field B threading a cavity within a superconductor which rotates at angular velocity ω , is given by $eB = 2(m \text{ sub } 0) - W/(c \text{ squared}) \omega$, where $-e$ is the charge on the electron, $(m \text{ sub } 0)$ is the free electron mass, W is the work-function of the superconductor, and c is the velocity of light. In the calculation effects which are second-order in the rotation velocity have been ignored, and the result is only strictly valid at the zero of temperature. The application of this result to experiments using practical, non-ideal apparatus is then illustrated for a simple geometry.

501,422
PB85-187284 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Mechanisms for Inception of DC and 60-Hz AC Corona in SF₆.
Final rept.,
R. J. Van Brunt, and M. Misakian. 1982, 15p
Sponsored by Department of Energy, Washington, DC. Div. of Electric Energy Systems.
Pub. in Proceedings of Conference on Electr. Insul. and Dielectr. Phenom., Symposium on Corona and Non-Spark Discharges, October 26-28, 1981, IEEE Trans. Electr. Insul. 17, n2 p106-120 Apr 82.

Keywords: *Sulfur hexafluoride, *Electric corona, Avalanche breakdown, Ionization, Measurement.

Using a pulse counting technique, inceptions of positive and negative point-plane corona in SF₆ under dc and 60-Hz ac conditions were measured. Effects of gas pressure, uv-radiation, and point electrode size on differences between ac and dc, and between positive and negative inceptions were investigated. Inceptions were also calculated using the streamer criterion. Agreement was obtained with measured negative inceptions for both ac and dc conditions, but not with positive inceptions. The growth in the active-electron initiation volume with applied voltage was calculated and used to explain the observed polarity effect. The magnitude of the polarity effect is predictably reduced either by irradiating the gap or by increasing the diameter of the point electrode.

501,423
PB85-197481 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Support-Electrode Torque on a Spherical Superconducting Gyroscope.
Final rept.,
L. B. Holdeman, and J. T. Holdeman. 1984, 6p
See also DE82-017519.
Pub. in IEEE (Institute of Electrical and Electronics Engineers) Transactions on Magnetism 20, n5 p2042-2047 1984.

Keywords: *Gyroscopes, *Superconductors, *Torque, *Relativity, Magnetic fields, Rotation, Boundary value problems, Reprints.

A rotating superconductor generates a magnetic field which can be used as a gyroscope readout. However, the Meissner effect of superconducting support electrodes will produce a torque. That torque is calculated in this paper.

501,424
PB85-205797 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Role of Photodetachment in Initiation of Electric Discharges in SF₆ and O₂.
Final rept.,
R. J. Van Brunt, and M. Misakian. 1983, 6p
Sponsored by Department of Energy, Washington, DC. Pub. in Jnl. of Applied Physics 54, n6 p3074-3079 Jun 83.

Keywords: *Electric discharges, *Sulfur hexafluoride, Oxygen, Avalanche breakdown, Reprints, Photodetachment.

The role of photodetachment in the initiation of electron avalanches near a positive point electrode was investigated using radiation between 295 and 630 nm from a chopped, tunable cw laser or filtered Hg-discharge lamp for a gap in which the negative ion flux was controlled by uv-irradiation of the cathode. Consistent with estimates based on known cross sections, photodetachment for light beams up to 500 mW was found to make a negligible contribution to avalanche initiation in SF₆ and O₂ at pressures from 50 to 500 kPa. The conditions under which photodetachment might be observed are discussed, and it is shown that for the conditions considered here, the expected dominant electron release mechanism in the gap is through collisional detachment of stable negative ions. Previously reported enhancements in avalanche rates resulting from irradiation of a positive point can be explained as arising from increases in negative ion densities due to attachment of photoelectrons ejected by scattered radiation.

501,425
PB85-230712 Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div.
Electromechanical and Metallurgical Properties of Liquid-Infiltration Nb-Ta/Sn Multifilamentary Superconductor.
Final rept.,
J. W. Ekin, and M. Hong. Aug 84, 4p
Sponsored by David W. Taylor Naval Ship Research and Development Center, Bethesda, MD.
Pub. in Applied Physics Letters 45, n3 p297-299, 1 Aug 84.

Keywords: *Superconductors, Critical field, Niobium, Tantalum, Tin, Reprints, Critical current.

Data are presented on the strain dependence of the critical current and critical field of Nb-Ta/Sn superconductors fabricated by the liquid Sn infiltration process. The results show that liquid infiltrated Nb-Ta/Sn superconductors have several significant advantages over bronze-process Nb/Sn superconductors: an overall ($J \text{ sub } c$) that is 3-10 times higher for magnetic fields in the range 13-20 T, an irreversible (damage) strain limit twice as large, and a ($J \text{ sub } c$) elastic-strain sensitivity less than half as large at fields above about 16 T. These improved properties are attributed to several unique characteristics of the liquid infiltration process: a tough Nb-Ta matrix, fine equiaxial A15 grains, and a uniform stoichiometric Sn concentration.

501,426
PB86-100690 PC A02/MF A01
National Bureau of Standards, Gaithersburg, MD.
Units for Magnetic Properties.
Mar 85, 3p NBS/SP-696
Also available from Supt. of Docs as SN003-003-02668-9.

Keywords: *Units of measurement, *Magnetic properties.

Column headings include the following: Quantity; Symbol; Gaussian and cgs emu; Conversion factor; SI and rationalized mks.

501,427
PB86-119427 Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div.
Hysteretic Losses in Nb-Ti Superconductors.
Final rept.,
R. B. Goldfarb, and A. F. Clark. Apr 85, 3p
Sponsored by Air Force Office of Scientific Research, Bolling AFB, DC.
Pub. in Jnl. of Applied Physics 57, n1 p3809-3811, 15 Apr 85.

Keywords: *Superconductors, *Magnetic hysteresis, Hysteresis, Magnetization, Niobium, Titanium, Losses, Reprints.

When subjected to transient magnetic fields, superconductors exhibit losses. At low frequencies, most of the dissipation is hysteretic. Magnetization was measured in an axial field for eight multifilamentary Nb-Ti superconducting wires with different filament sizes and different ratios of copper to superconductor. The full-penetration field $H(p)$ was estimated from the high-field ends of the hysteresis loops. The estimate of $H(p)$

provides a method to assess the critical current density J_c . There was good agreement between measured losses and those predicted from $H(p)$ and the peak applied field.

501,428
PB86-128972 Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Fields Div.
Multisensor Automated EM (Electromagnetic) Field Measurement System.
Final rept.,
W. Bensema, G. Reeve, and G. Koepke. 1985, 3p
Pub. in Proceedings of Institute of Electrical and Electronics Engineers 1985 Instrumentation and Measurement Technology Conference, Tampa, FL., March 20-22, 1985, p200-202.

Keywords: *Electromagnetic fields, *Measurement, Reverberation, Monitors.

A system is being developed to monitor and collect electromagnetic (EM) field strength at multiple locations simultaneously. The system has two modes of operation: (1) for sampling EM fields that are stationary for times of the order of 200 ms, and (2) for sampling changing EM fields with a system resolution of 10 micro seconds.

501,429
PB86-129491 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Electrical Measurements and Standards Div.
Design and Construction of a Superconducting Magnet System for the Absolute Ampere Experiment.
Final rept.,
W. Y. Chen, J. R. Purcell, P. T. Olsen, W. D. Phillips, and E. R. Williams. 1982, 8p
Pub. in Advances in Cryogenic Engineering 27, p97-104 1982.

Keywords: Superconducting magnets, Magnetic fields, Electric current, Standards, *Superconducting coils, *Ampere.

The Electrical Measurements and Standards Division of the National Bureau of Standards will undertake an absolute ampere experiment, which will involve measuring the force exerted on a current-carrying, normal conductor coil by a set of superconducting coils and also measuring the voltage induced in the normal coil as it is moved in the field of the superconducting coils. To achieve the desired accuracy and resolution, the superconducting coils are required to generate nearly purely radial fields of about 0.2 tesla at a radius of 35 cm, over a region of $\Delta R = + \text{ or } - 0.8 \text{ cm}$ and $\Delta Z = + \text{ or } - 2.5 \text{ cm}$. The quality of the field is represented by the product $r(\text{dot})(B \text{ sub } r)$ which must be held uniform within 20 ppm over the specified region.

501,430
PB86-167327 PC A04/MF A01
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Fields Div.
Possible Estimation Methodologies for Electromagnetic Field distributions in Complex Environments.
Technical note,
M. Kanda, J. Randa, and N. S. Nahman. Mar 85, 52p NBS/TN-1081

Keywords: *Electromagnetic fields, Distribution, Estimating, Environments, Hazards, Scanning, Statistical analysis.

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 outlines three general approaches to the problem which are currently under investigation at the National Bureau of Standards. The three approaches are: (1) a statistical treatment of the spatial distribution of electromagnetic field intensities; (2) a numerical computation using a finite-difference (or lattice) form of the electromagnetic action functional; and (3) use of a directional probe to scan a volume. All three methods are still in the development stage, but each appears promising.

Field 20—PHYSICS

Group 20D—Fluid Mechanics

20D. Fluid Mechanics

501,431
PB85-170629 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Flow and Temperature Profile Independence of Flow Measurements Using Long Acoustic Waves.
Final rept.,
B. Robertson. Mar 84, 3p
Pub. in Jnl. of Fluids Engineering 106, p18-20 Mar 84.
Keywords: *Flow measurement, *Elastic waves, Sound transmission, Velocity, Pipes(Tubes), Temperature, Frequencies, Reprints.

An expansion in powers of V/c is derived for the wave number of the fundamental sound mode in a flow conduit, where V is the velocity of fluid in the conduit and c is the local sound speed. Both V and c are assumed to be independent of the longitudinal coordinates and of the time, but may have arbitrary profiles. The calculation applies to frequencies well below the cutoff frequency of the conduit, which may have an arbitrary cross-sectional shape. To lowest order, the wave number depends only on the average of the longitudinal component of V and is independent of its profile.

501,432
PB85-184661 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Numerical-Experimental Study of Confined Flow Around Rectangular Cylinders.
Final rept.,
R. W. Davis, E. F. Moore, and L. P. Purtell. 1984, 14p
Pub. in Physics of Fluids 27, n1 p46-59 Jan 84.

Keywords: *Fluid flow, *Cylinders, Experimentation, Numerical analysis, Aspect ratio, Blocking, Velocity, Pressure, Reynolds number, Mathematical models, Wind tunnels, Tests, Vortices, Computerized simulation, Unsteady flow, Containment, Reprints, *Vortex shedding, Strouhal number, Numerical flow visualization.

A previous numerical study by Davis and Moore of vortex shedding from rectangles in infinite domains is extended to include the effects of confining walls. The major changes to the numerical modeling are the addition of a direct solver for the pressure equation and the use of an infinite-to-finite mapping downstream from the rectangle. The parameters in the problem are now Reynolds number, rectangle aspect ratio, blockage ratio, and upstream velocity profile. As each of these is varied, the effects upon the forces acting on the rectangle and the structure of the wake are discussed. Streakline plots composed of multishaped passive marker particles provide a clear visualization of the vortices. These plots are compared with smoke-wire photographs taken from a wind tunnel test. Strouhal numbers obtained both computationally and experimentally are compared for two values of the blockage ratio. Moving recirculation zones which appear between the wake and the walls are discussed.

501,433
PB85-197457 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Numerical Solutions for a Moving Shear Layer in a Swirling Axisymmetric Flow.
Final rept.,
H. Baum, M. Ciment, R. W. Davis, and E. F. Moore. 1981, 485p
Pub. in Proceedings of International Conference on Numerical Methods in Fluid Dynamics (7th), Lecture Notes in Physics Series 141, 485p 1981.

Keywords: *Axisymmetric flow, Viscous flow, Unsteady flow, Incompressible flow, Reynolds number, Swirling, Mathematical models, Numerical analysis, Fluid dynamics, *Shear layers, Cylindrical coordinates.

This paper presents both a new model problem for unsteady, incompressible viscous flow and a new numerical method for modeling flows in cylindrical geometries. The model problem is an exact solution to the fully three-dimensional axisymmetric Navier-Stokes equations and is shown to represent a moving shear layer of rotating fluid whose thickness depends on Reynolds number. An asymptotic steady-state is reached which consists of a potential vortex with a viscous core. The new numerical method is a fundamental solution technique for cylindrical coordinates similar in derivation to the El-Mistikawy-Werle scheme (AIAA J., 16, p. 749, 1978) for cartesian coordinates. This

method is implemented in the context of the operator compact implicit (OCI) format. The new scheme and several others are tested on the model problem over a range of Reynolds numbers.

501,434
PB85-197531 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Magnetohydrodynamics of Laminar Flow in Slowly Varying Tubes in an Axial Magnetic Field.
Final rept.,
J. M. McMichael, and S. Deutsch. 1984, 9p
Pub. in Physics of Fluids 27, n1 p110-118 Jan 84.

Keywords: *Magnetohydrodynamics, *Laminar flow, *Pipe flow, Reprints.

Laminar flow of a conducting fluid in round, straight tubes with axially varying radius, with a uniform magnetic field applied parallel to the tube axis, is treated theoretically as a regular perturbation problem at finite hydrodynamic Reynolds number, finite magnetic Reynolds number, and Hartmann numbers as large as $O(\alpha \sup -1/2)$, where α is a small parameter characteristic of the slope of the tube wall. The first order solution is examined numerically for local tube dilations and for local constrictions. Flow separation along both converging and diverging sections of the tube is explored in detail. Pressure, current density, and induced magnetic field distributions are also presented.

501,435
PB85-230761 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Numerical Simulation of Flow Around Squares.
Final rept.,
R. W. Davis, and E. F. Moore. 1981, 13p
Pub. in Proceedings of the International Conference on Numerical Methods in Laminar and Turbulent Flow (2nd), Venice, Italy, July 13-16, 1981, p279-290.

Keywords: *Computerized simulation, *Two dimensional flow, *Unsteady flow, Reynolds number, Velocity, Lift, Drag, Aerodynamic configurations, Finite difference theory, Numerical analysis, Fluid mechanics, Aerodynamics, Mathematical models, Convection, *Square configuration, Strouhal number, Vortex shedding.

The paper presents a numerical simulation of two-dimensional unsteady flow around squares in infinite domains with uniform upstream velocity profiles. Variations in the behavior of lift and drag with Reynolds number are discussed. Passive marker particles are used to visualize the onset and subsequent development of vortex shedding at a Reynolds number of 1000. The finite difference scheme employed in this simulation utilizes third-order accurate upwind differencing for convection and a Leith-type of temporal differencing. Variations in convective differencing near the corners of the square and at the out-flow boundary of the mesh are described.

501,436
PB86-128238 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Fluid Engineering Div.
Drag on a Sphere Moving Horizontally Through a Stratified Liquid.
Final rept.,
K. E. B. Lofquist, and L. P. Purtell. 1984, 14p
Sponsored by Office of Naval Research, Arlington, VA.
Pub. in Jnl. of Fluid Mechanics 148, p271-284 Nov 84.

Keywords: *Drag, *Spheres, Salt water, Wakes, Reprints, Stratified flow, Stratified fluids.

The drag on a sphere moving horizontally through stably stratified salt water is measured in laboratory experiments. The increment in drag coefficient due to the stratification, ΔC_D , is obtained as function of a stratification parameter, κ (eq. 5) and, in principle, the usual Reynolds number, R . In these experiments, where R ranges from 150 to 5,000, ΔC_D is insensitive to R . But as function of κ , ΔC_D has both positive and negative values. A positive peak in $\Delta C_D(\kappa)$, about as large as the unstratified C_D , is identified as a resonance maximum in the lee-wave drag. Negative values of $\Delta C_D(\kappa)$, as large as 15% of C_D , are interpreted as a reduced rate of generation of heat within the wake due to inhibition of vertical turbulent motions and vertical spreading of the wake by the stable stratification.

501,437

PB86-136728 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Chemical Process Metrology Div.
Numerical Modeling of Unsteady Gas-Particle Flows Around Rectangles Inside Channels.
Final rept.,
R. W. Davis, E. F. Moore, and C. T. Crowe. 1983, 10p
Pub. in Proceedings of International Conference on Numerical Methods in Laminar and Turbulent Flow (3rd), Seattle, WA., August 8-11, 1983, p1037-1046.

Keywords: *Gas flow, Mathematical models.

The paper presents numerical solutions for gas-particle flows around rectangles inside two-dimensional channels. Vortex shedding frequencies are seen to compare well with the results of a wind tunnel experiment. Trajectories of individual physical particles through this highly unsteady flow are presented for varying combinations of Stokes number and gravitational force. The numerical scheme utilizes an explicit Leith-type of temporal differencing and quadratic upwind differencing for convection.

501,438

PB86-136736 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Chemical Process Metrology Div.
Finite Difference Methods for Fluid Flow.
Final rept.,
R. W. Davis. 1984, 19p
Pub. in Proceedings of 1983 International Conference on Computational Techniques and Applications: CTAC-83, University of Sydney, Australia, August 28-31, 1983, p51-69 1984.

Keywords: *Navier-Stokes equations, *Finite difference theory, Unsteady flow, Computerized simulation, *Computational fluid dynamics, Separated flow.

The purpose of the paper is to describe how finite difference methods can be employed to solve the incompressible Navier-Stokes and continuity equations of fluid flow. The differencing of the various terms in these equations is considered in detail, and a solution procedure is presented which gives reasonable results for two complex flow problems. These problems involve unsteady viscous separated flows in the wake of a rectangular obstacle inside a two-dimensional channel and in an axisymmetric mixing layer. The importance of a priori testing of the numerical methods on appropriate simple model problems is stressed and a useful example is given. Also stressed is the importance of computational flow visualization and data analysis in order to make sense of a flow calculation.

501,439

PB86-154036 PC A03/MF A01
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Chemical Engineering.
Experimental/Computational Investigation of Organized Motions in Axisymmetric Coflowing Streams.
Final rept.,
R. W. Davis. Dec 85, 40p NBSIR-85/3287
Sponsored by Air Force Office of Scientific Research, Bolling AFB, DC.

Keywords: *Entrainment, Jet flow, Axisymmetric flow.

A joint experimental/computational investigation of the entrainment process in the turbulent mixing of a round jet with a coflowing stream has been carried out. The overall objectives of this work were to identify and characterize coherent motions in the mixing region, investigate the dynamical role these motions play in the entrainment process, and determine the extent to which entrainment is affected by such factors as initial conditions and forcing.

20E. Masers and Lasers

501,440

PB85-201820 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Center for Basic Standards.

Single-Shot Spectral Measurements and Mode Correlations in a Multimode Pulsed Dye Laser.

Final rept.,
W. A. Westling, M. G. Raymer, and J. J. Snyder. Apr 84, 5p
Contract DE-AC02-ER10797
Pub. in Jnl. of the Optical Society of America B 1, n2 p150-154 Apr 84.

Keywords: *Light pulses, Correlations, Intensity, Reprints, Dye lasers, Pulsed lasers, Hole burning, Multimode.

Statistical cross correlations between mode intensities in individual pulses from a multimode dye laser have been studied using a Fizeau interferometer and a high resolution linear photodiode array. It was found that positive intensity cross correlations develop between modes separated by certain characteristic frequencies. This appears to be a result of spatial hole burning in the standing-wave cavity. The gain competition between certain modes is minimized due to the spatial inhomogeneity of the mode intensity distributions in the gain medium.

501,441
PB85-202802 Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Electromagnetic Technology Div.
Calorimeter for Measuring 1-15 kJ Laser Pulses.
Final rept.,
P. A. Simpson, and E. G. Johnson. 1984, 4p
Pub. in Proceedings of SPIE - Optical Radiation Measurements, San Diego, CA., August 21-22 1984, p121-124.

Keywords: *Calorimeters, *Power measurement, Laser beams, *Laser radiation, Pulsed lasers.

Two calorimeters for measuring high peak power laser pulses have been constructed by the NBS and delivered to the Newark Air Force Station, Newark, Ohio. These calorimeters are designed to measure pulses having intensities great enough to damage the volume absorbing material in normal calorimeters. In these new calorimeters, the volume absorbing material is already fragmented and flowing dry N₂ gas is used to extract the temperature rise information. Pulse energy can be in the range 1 to 15 kJ. Wavelength range is from the ir to uv by employing various volume absorbing materials.

501,442
PB85-206647
(Order as PB85-206324, PC A13/MF A01)
Academia Sinica, Shanghai (China). Shanghai Inst. of Optics and Fine Mechanics.
Raman Spectra of LiYF₄ Crystal.
F. Y. Gan, and H. Y. Chen. Apr 85, 3p
Included in OM85: Basic Properties of Optical Materials. Summaries of Papers, p130-132 Apr 85.

Keywords: *Laser materials, *Raman spectra, Infrared lasers, Neodymium, *Lithium yttrium fluorides, Doped materials, Tunable lasers, Optical phonons, Polarization.

Rare earth ion doped LiYF₄ crystals are well-known laser active materials; they produce the laser emissions in the range of 0.8-2.1 micrometer wavelength. LiYF₄ host structure, a scheelite model, is a body-centre tetragonal with $a = 5.175\text{ \AA}$ and $c = 10.74\text{ \AA}$. The polarized fluorescence and absorption, excitation spectra, life-time, etc. of the crystal doped with Nd(3+) have been studied in detail and the crystal-field parameters have also been reported, but only a few works about its vibrational properties have been presented so far. The optical phonon spectra are rather important for development of tunable solid state lasers; for this reason the authors carried out the study of Raman spectra of this material, analyzed its optical mode vibrations, and finally compared with that of the sample doped with Nd(3+).

501,443
PB85-206746
(Order as PB85-206324, PC A13/MF A01)
Nebraska Univ., Lincoln. Dept. of Electrical Engineering.
Optical Properties of Ion Beam Irradiated Molybdenum Laser Mirrors as Studied by Ellipsometry.
J. A. Woollam, G. H. Bu-Abbud, D. L. Mathine, D. Poker, and D. Ingram. Apr 85, 2p
Prepared in cooperation with Oak Ridge National Lab., TN., and Universal Energy Systems, Dayton, OH.
Included in OM85: Basic Properties of Optical Materials. Summaries of Papers, p167-168 Apr 85.

Keywords: *Mirrors, *Molybdenum, Surface roughness, Polarimetry, Reflectivity, *Laser mirrors, Ellipsometry, Ion implantation, Refractive index, Extinction coefficients.

In this paper the authors report on implantation of Mo ions into polished molybdenum surfaces to investigate the effects of implantation on surface roughness, and optical reflectivity. The motivation is to develop ion beam techniques for improving the reflectivity and (surface smoothness) over a wide spectral range. Information on the index of refraction and extinction coefficient as functions of wavelength are also obtained.

501,444
PB85-206753
(Order as PB85-206324, PC A13/MF A01)
Anhui Inst. of Optics and Fine Mechanics (China).
Crystal Field Energy Levels and Optical Absorption Intensities of Ni(2+):MgF₂.
B. Zhang, J. K. Zhu, and S. H. Liu. Apr 85, 2p
Included in OM85: Basic Properties of Optical Materials. Summaries of Papers, p169-170 Apr 85.

Keywords: *Laser materials, *Magnesium fluorides, *Energy bands, Nickel, Atomic energy levels, Magnetic dipoles, Absorbance, *Crystal field, Oscillator strengths, Nickel ions.

One-electron energy levels and wave functions of laser crystal Ni(2+):MgF₂ with lower symmetric crystal fields (D sub (2 sup h)) are calculated by use of the spin-unrestricted MS-X(alpha) method.

501,445
PB85-206795
(Order as PB85-206324, PC A13/MF A01)
Vanderbilt Univ., Nashville, TN. Dept. of Physics and Astronomy.
Surface Erosion Induced by Electronic Transitions.
R. F. Haglund, and N. H. Tolk. Apr 85, 4p
Included in OM85: Basic Properties of Optical Materials. Summaries of Papers, p184-187 Apr 85.

Keywords: *Ultraviolet optical materials, *Radiation damage, Synchrotron radiation, Electron irradiation, Surfaces, Erosion, Sodium chloride, Lithium fluorides.

The problem of damage to ultraviolet optical materials has been and continues to be a major source of concern in the design and operation of high-power lasers. Little fundamental understanding exists of the atomic-level mechanisms which operate to produce this damage. However, recent experiments have shown that irradiation of optical materials by electrons and photons at energies characteristic of high-power and high-energy laser systems is an efficient cause of surface erosion. The experiments described here are intended to illuminate the basic mechanisms associated with energy absorption, distribution and localization leading to electronically induced desorption, and to determine the role of defects in these processes.

501,446
PB85-207231 Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
External Dye-Laser Frequency Stabilizer.
Final rept.,
J. L. Hall, and T. W. Haensch. Nov 84, 3p
Contract NSF-PHY82-00805
Pub. in Optics Letters 9, n11 p502-504 Nov 84.

Keywords: *Frequency stability, Phase modulation, Electrooptics, Reprints, *Dye lasers, Acoustooptics.

The authors describe an external dye laser frequency stabilizer, that combines an acoustooptic frequency shifter with a fast electro-optic phase modulator. A compensating electronic delay line in the crossover network provides a near-ideal transducer response, while keeping the voltage across the electro-optic crystal away from the amplifier limits.

501,447
PB86-103017 Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Time and Frequency Div.
Efficient Single Mode Operation of a CW Ring Dye Laser with a Mach-Zehnder Interferometer.
Final rept.,
J. C. Bergquist, and L. Burkins. Jul 84, 7p
Sponsored by Air Force Office of Scientific Research, Bolling AFB, DC., and Office of Naval Research, Arlington, VA.

Pub. in Optics Communications 50, n6 p379-385, 15 Jul 84.

Keywords: Reprints, *Dye lasers, *Ring lasers, Continuous wave lasers, Mach-Zehnder interferometers.

Stable single mode operation of a ring dye laser is obtained with the combination of a Mach-Zehnder interferometer (MZI), three plate birefringent filter, a single thin etalon, and a unidirectional diode. The MZI eliminates the fractional insertion loss due to beam walk-off and distortion which an intracavity etalon must introduce in order to select single frequency operation. The authors experimentally demonstrate the low insertion loss, single mode stability, and frequency tuning of a ring dye laser using a specially designed, compact MZI. Finally, the authors propose MZIs with no coatings, which should permit extremely low loss broadband operation.

501,448
PB86-140225 Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Time and Frequency Div.
New Miniaturized Passive Hydrogen Maser.
Final rept.,
F. L. Walls, and K. B. Persson. 1984, 4p
Sponsored by Naval Research Lab., Washington, DC.
Pub. in Proceedings of the Frequency Control Symposium (38th), Philadelphia, Pennsylvania, May 29-June 1, 1984, p416-419.

Keywords: *Masers, Frequency stability, Cesium frequency standards, Time standards, *Hydrogen masers.

The small passive hydrogen maser design developed at NBS has been further refined to produce a much smaller device with enhanced performance. This new miniaturized passive hydrogen maser is rack mounted, measuring 26 1/2 cm high exclusive of its external power supply. The weight is about 30 kgm with a steady state power consumption of about 54W at 25C. The reduction in the size and power has been achieved primarily by major changes in the beam optics, offset frequency synthesizer, and hydrogen supply. The present size is small enough to fit in the NBS environmental chamber used to house commercial cesium frequency standards.

20F. Optics

501,449
PB85-170611 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Absolute Spectral Irradiance Measurements Based on the Predicted Quantum Efficiency of a Silicon Photodiode.
Final rept.,
E. F. Zalewski, and W. K. Gladden. 1984, 8p
Pub. in Optica Pura Y Aplicada 17, n2 p133-140 1984.

Keywords: *Irradiance, Optical measurement, Spectroradiometers, Photodiodes, Quantum efficiency, Silicon, Helium neon lasers, Reprints, Laser applications.

The spectral irradiance of an incandescent lamp was measured with a grating spectroradiometer that was calibrated at 632.8 nm with a HeNe laser and an absolute detector. The absolute detector was a silicon photodiode whose response was determined by the predictable quantum efficiency (also known as self-calibration technique). These results were compared to the spectral irradiance values obtained by calibrating the lamp relative to a black-body source traceable to the freezing point of gold. The ratio of the black-body based irradiance to detector based irradiance was found to be 1.0075 within a combined uncertainty of + or - 1.12%.

501,450
PB85-183507 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Photodiode Quantum Efficiency Enhancement at 365 nm: Optical and Electrical.
Final rept.,
R. L. Booker, and J. Geist. 1982, 3p
Pub. in Applied Optics 21, n22 p3987-3989 1982.

Keywords: *Photodiodes, *Quantum efficiency, Near ultraviolet radiation, Oxides, Silicon, Reprints.

Field 20—PHYSICS

Group 20F—Optics

Prolonged exposure of oxide-p(+)-n-n(+) silicon photodiodes to ultraviolet radiation increases their quantum efficiency. The cause of this effect is shown to be the storage of photogenerated negative charge at the front surface of the oxide.

501,451
PB85-184828 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Comment on Representation of Vector Electromagnetic Beams.

Final rept.,
L. W. Davis, and G. Patsakos. 1982, 2p
Pub. in Physical Review A 26, n6 p3702-3703 Dec 82.

Keywords: *Laser beams, Reprints, Whittaker potentials.

The omission of a class of beam modes by Pattanayak and Agrawal is rectified, and the relationship of the representation of electromagnetic beams used by them to that used by the present authors is clarified.

501,452
PB85-187557 PC A03/MF A01
National Bureau of Standards, Gaithersburg, MD.
Modulation Transfer Function for Two-Point and Periodic Objects Using Gaussian and Lorentzian Resolution Functions.

Interim rept.,
R. A. Scrack. Jun 84, 35p NBSIR-84/2893
Sponsored by Department of Energy, Washington, DC.

Keywords: *Resolution, Neutron radiography, Normal density functions, *Modulation transfer functions, Imaging techniques, One dimensional.

This paper presents an analytical study of the effect of Gaussian- and Lorentzian-shaped line spread functions in non-coherent noise-free imaging systems. A mathematic development is given for the calculation of the Modulation Transfer Function (MTF). This technique is used to calculate the MTF for two-point and periodic objects using Gaussian and Lorentzian resolution functions. Figures and graphs are used to illustrate the comparison of the results. Relationships between the results obtained are developed that are useful in the interpretation of experiments used to determine the resolution of experimental systems. The development covers only noise-free, incoherent, one-dimensional systems.

501,453
PB85-189355 Not available NTIS
National Bureau of Standards (NML), Boulder, CO.
Quantum Physics Div.
Configuration Interaction in Multiphoton Ionization.

Final rept.,
P. Zoller, E. Matthias, and S. J. Smith. 1984, 9p
Grants NSF-PHY82-00805, NSF-INT81-20128
Pub. in Proceedings of NAGO Summer School in Quantum Electrodynamics and Quantum Optics, Boulder, CO, May 26-June 8, 1983, p313-321 1984.

Keywords: *Photoelectrons, Angular distribution, Ionization, *Barium atoms, *Configuration interaction, *Multiphoton ionization.

The application of multichannel quantum-defect theory (MQDT) to interpretation of recent photoelectron angular distribution measurements obtained in this laboratory by resonant multiphoton excitation and ionization of atomic barium, is discussed. The pronounced effect of a doubly excited (5d7d) state acting to perturb the singly excited 6snd Rydberg series makes these angular distributions and their interpretation particularly significant.

501,454
PB85-194736 PC A03/MF A01
National Bureau of Standards (NEL), Boulder, CO.
Electromagnetic Technology Div.
Redefining the Scratch Standards.

M. Young, and E. G. Johnson. Feb 85, 28p NBS/TN-1080
Sponsored by Army Armament Research and Development Command, Dover, NJ. Also available from Supt. of Docs as SN003-003-02635-2.

Keywords: *Optical measurement, *Standards, *Surfaces, Diffraction, Gratings(Spectra), Surface properties, *Scratch standards, MIL standards.

The scratch standard (MIL-0-13830A) is a cosmetic standard that is effected by a visual comparison with a

set of submasters that are in turn evaluated by comparison with a set of master standards. Both manufacture and certification of the submasters are somewhat unreliable. In this paper, the authors show that the submasters can be classified according to the relative power scattered at a relatively small angle. They have designed etched gratings with which to replace the submasters; these gratings have the appearance of scratches but diffract a broad peak between 5 and 10 degrees off the axis of the incident beam. The authors have classified some prototypes both by comparison with the master standards and by a photoelectric measurement; agreement between the two methods is good. The authors suggest that such gratings be used as the submasters and possibly that they be classified by a photoelectric rather than visual measurement.

501,455
PB85-195303 PC A03/MF A01
National Bureau of Standards, Gaithersburg, MD.
Self-Study Manual on Optical Radiation Measurements. Part 1. Concepts. Chapter 12. Blackbodies, Blackbody Radiation, and Temperature Scales.

Technical rept.,
J. C. Richmond, and F. E. Nicodemus. Apr 85, 49p
NBS/TN-910-8
See also PB84-218346. Also available from Supt. of Docs as SN003-003-02647-6.

Keywords: *Optical measurement, *Radiometry, *Blackbody radiation, *Temperature, *Thermal radiation, Temperature measurement, Manuals, Fundamental constants, Thermodynamics, Plancks constants, Stefan-Boltzmann equation.

This is the eighth in a series of Technical Notes (910-) entitled 'Self-Study Manual on Optical Radiation Measurements'. It contains Chapter 12 of Part I of this Manual. Additional chapters will continue to be published, similarly, as they are completed. The Manual is a comprehensive tutorial treatment of the measurement of optical radiation that is complete enough for self-instruction. Detailed chapter summaries make it also a convenient authoritative reference source. In this chapter, the authors review the radiometric treatment, and the significance for radiometric measurements, of blackbodies, blackbody radiation, and temperature scales. Many important and interesting aspects are not treated because the authors primary interest is in radiometry and radiometric measurements. The emphasis is on ideal blackbodies and laboratory simulators; thermal radiation from other real sources will be treated in a chapter on Thermal Radiation Properties of Materials.

501,456
PB85-195923 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
What is Dynamic Dispersion.

Final rept.,
J. Reader. 1981, 2p
Pub. in Applied Optics 20, n13 p2171-2172, 1 Jul 81.

Keywords: *Optical dispersion, Gratings(Spectra), Reprints, *Dynamic dispersion, *Dispersion.

It is shown that the quantity dynamic dispersion, introduced by Lockwood in 1973, does not differ from ordinary dispersion.

501,457
PB85-195980 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Radiometry Using Synchrotron Radiation.

Final rept.,
E. B. Saloman, S. C. Ebner, and L. R. Hughey. 1981, 8p
Sponsored by SPIE-The International Society for Optical Engineering, Bellingham, WA.
Pub. in Proceedings of the SPIE 279, Washington, DC., April 21-22, 1981, p76-83.

Keywords: *Synchrotron radiation, *Ultraviolet radiation, *Radiometry, *Calibrating, X rays, Storage rings, Uncertainty.

Synchrotron radiation is a source of continuum radiation ranging from the x-ray or soft x-ray region (depending on machine energy) to beyond the visible region. The amount of radiation emitted is a calculable function of machine operating parameters. This makes it possible to use synchrotron radiation from electron synchrotrons and electron storage rings as an absolute source particularly in the VUV and soft x-ray regions where other standards are difficult to find. At the National Bureau of Standards (NBS) an electron stor-

age ring (SURF-II) has been used to calibrate spectrometers and photometers used in solar and aeronomy research and in fusion plasma diagnostics. A large chamber has recently been completed to facilitate such calibrations. The radiation incident on these spectrometers can be calculated to uncertainties of 3%. A technique to exactly determine the number of electrons orbiting in the ring is currently being developed to reduce this uncertainty.

501,458
PB85-196012 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Optical Bistability Experiments and Mean Field Theories.

Final rept.,
W. J. Sandle, R. J. Ballagh, and A. Gallagher. 1981, 16p
Pub. in Proceedings of International Conference on Optical Bistability, Ashville, NC., June 3-5, 1980, p93-108 1981.

Keywords: *Optical bistability, Laser radiation.

Theories of optical bistability have largely been concerned with idealized two-state absorbers in optical cavities, but experiments must contend with the properties of real atoms. The main purpose of this paper is to present experimental evidence for optical bistability taken under conditions where real atomic behavior can be closely represented by the two-state model, so that tests of mean field theories of OB are possible. An important feature of the work is the use of high optical intensities obtained with a near-concentric focussing cavity.

501,459
PB85-200186 PC A04/MF A01
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Mfg. Engineering.
Transient Analysis of Electromagnetic Reflection from Dispersive Materials.

A. G. Lieberman. Mar 85, 73p NBS/TN-1202
Also available from Supt. of Docs as SN003-003-02651-4.
Keywords: *Light pulses, Plane waves, Polarization(Waves), Greens function, Surfaces, *Electromagnetic wave reflections, Laser radiation, Drude model, Transients, Dispersion, Femtosecond pulses.

Theoretical expressions are presented describing the transient and steady-state temporal evolution of an impulsive, TE-polarized, plane wave reflected into vacuum from any of a variety of frequency-dispersive material surfaces. Polar dielectrics, non-polar dielectrics, metals and plasmas are treated using, respectively, the Debye, Lorentz, and Drude material models to investigate the effects of dispersion upon dimensional measurements performed with optical pulses of extremely short duration. The more general problem, concerning the reflection of an optical pulse of any specified waveform, is resolved by performing a convolution of the incident wave at the material surface with the previously determined reflection of an impulsive wave.

501,460
PB85-205284 Not available NTIS
National Bureau of Standards (NEL), Boulder, CO.
Electromagnetic Technology Div.
Detectors for Picosecond Optical Power Measurements.

Final rept.,
R. J. Phelan, D. R. Larson, N. V. Frederick, and D. L. Franzen. 1984, 4p
Pub. in Proceedings of SPIE, Optical Radiation Measurements, San Diego, CA., August 21-22, 1984, v499 p34-37.

Keywords: *Light pulses, *Power measurement, *Optical measuring instruments, Photodiodes, Silicon, *Picosecond pulses, Schottky barrier devices, Silicon on sapphire, Laser radiation.

There are many features in addition to time resolution that are desirable for a picosecond optical power measurement system. An interdigitated contact, Schottky barrier silicon photodiode coupled to an electro-optic sampler exhibits a rise time better than 22 picoseconds, a quantum efficiency greater than 30%, a uniform responsivity over its receiving aperture, and a usable spectral response to beyond 2 micrometers.

501,461
PB85-205623 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Effect of Atmospheric Attenuation on Temperature Measurements Made Using Infrared Scanning Systems.

Final rept.,
T. P. Sheahen. 1983, 8p
Pub. in Applied Optics 22, n7 p1070-1077, 1 Apr 83.

Keywords: *Atmospheric attenuation, *Infrared radiation, *Temperature measurement, Carbon dioxide, Water vapor, Reprints, *Atmospheric transmissivity, *Thermography, Remote sensing.

The atmosphere attenuates infrared radiation in the frequency range 3 - 5 micrometers even at distances as short as one meter. In order to do precise quantitative infrared thermography, it is necessary to correct the received signal for this attenuation. This paper develops a simple model and presents numerical calculations of the attenuation expected at a few meters distance, for one typical thermographic imaging system. (The extension to other equipment could easily be done by substituting different numerical data for the detector response.) The attenuation factors due to CO₂ and due to H₂O are 6% and 8%, respectively, at 10 meters range. A wide variety of target temperatures and ambient humidity conditions were examined; representative curves selected from this output are presented. Because of the importance of precise infrared measurements for industrial applications, the effect of varying CO₂ concentration was also studied.

501,462
PB85-206050 PC A04/MF A01
National Bureau of Standards (NML), Gaithersburg, MD. Center for Radiation Research.
Transmittance MAP (Measurement Assurance Program) Service.

Final rept.,
K. L. Eckerle, J. J. Hsia, and V. R. Weidner. Mar 85, 54p NBS/SP-692
Also available from Supt. of Docs as SN003-003-02655-7. Library of Congress catalog card no. 85-600513.

Keywords: *Transmittance, Accuracy, Filters, Wavelengths, Calibrating, Measurement, Spectrophotometers, Measurement Assurance program, Neutral density filters, Didymium filters, US NBS.

An introduction to the Transmittance Measurement Assurance Program (MAP) service is given. Documentation for the service is provided through a comprehensive list of references. The results of a pilot run for the MAP service are given in a sample calibration report.

501,463
PB85-206324 PC A13/MF A01
National Bureau of Standards, Gaithersburg, MD.
OM85: Basic Properties of Optical Materials. Summaries of Papers.

Final rept.,
A. Feldman. Apr 85, 297p NBS/SP-697
See also PB85-206332 through PB85-207025. Also available from Supt. of Docs as SN003-003-02648-4. Library of Congress catalog card no. 85-600534. Presented at the Topical Conference on Basic Properties of Optical Materials, National Bureau of Standards, Gaithersburg, Maryland, May 7-9, 1985. Sponsored by Air Force Office of Scientific Research, Bolling AFB, DC. and American Physical Society, Ne

Keywords: *Optical materials, *Meetings, Infrared optical materials, Ultraviolet optical materials, Optical glass, Polymers, Metals, Thin films, Fiber optics, Optical waveguides, Refractive index, Nonlinear optics, Photofractive effect, Semiconductors.

This Special Publication contains summaries of papers to be presented at the Topical Conference on Basic Properties of Optical Materials to be held at the National Bureau of Standards in Gaithersburg, Maryland on May 7-9, 1985. The conference is sponsored by the National Bureau of Standards, the Air Force Office of Scientific Research, and the American Physical Society in cooperation with the Optical Society of America and SPIE-The International Society for Optical Engineering. This publication contains summaries of 70 papers which include 17 invited papers. The purpose of the conference is to bring together researchers from industry, academia, and government to discuss the physical and structural properties of optical materials as they affect optical performance. The scope of the

conference includes the measurement and theory of basic properties of optical materials in bulk and in thin film form and the dependence of these properties on atomic structure, morphological structure, impurity content, and inhomogeneity.

501,464
PB85-206332 (Order as PB85-206324, PC A13/MF A01)
Bell Labs., Holmdel, NJ.

Progress in Optical Materials Research (Keynote Talk).
I. P. Kaminow. Apr 85, 4p
Included in OM85: Basic Properties of Optical Materials. Summaries of Papers, p1-4 Apr 85.

Keywords: *Optical materials, Fiber optics, Semiconductor lasers, Electrooptics, Reviews, Optical fibers, Nonlinear optics.

Topics discussed include optical fibers, semiconductor lasers, electrooptics and non-linear optics, and photonic structures.

501,465
PB85-206340 (Order as PB85-206324, PC A13/MF A01)
Bell Communications Research, Inc., Murray Hill, NJ.
Determination of Microstructure from Spectrophotometry and Spectroellipsometry.
D. E. Aspnes. Apr 85, 6p
Included in OM85: Basic Properties of Optical Materials. Summaries of Papers, p5-10 Apr 85.

Keywords: *Microstructure, *Spectrophotometry, Optical properties, Spectroellipsometry.

That microstructure can profoundly influence optical properties of materials has been known essentially from the first investigations of the electromagnetic response of macroscopic media. 'Microstructure' is used here in the standard materials science sense, referring to spatial inhomogeneities on the scale of about 1 to 25 nm. These are inhomogeneities large enough so that the separate regions possess their own dielectric identity, yet small compared to the wavelength of light. The present summary deals primarily with the modeling problem, and will cover topics that, in the opinion of the author, have not been adequately discussed elsewhere.

501,466
PB85-206357 (Order as PB85-206324, PC A13/MF A01)
Yale Univ., New Haven, CT.

Light Scattering from Dielectric and Metallic Microstructures.
R. K. Chang, and P. W. Barber. Apr 85, 6p
Prepared in cooperation with Clarkson Coll. of Technology, Potsdam, NY. Dept. of Electrical and Computer Engineering.
Included in OM85: Basic Properties of Optical Materials. Summaries of Papers, p11-16 Apr 85.

Keywords: *Light scattering, *Optical measurement.

The generalized Lorenz/Mie formalism can be used to calculate the elastic scattering (e.g., extinction and scattering cross sections) and the internal electromagnetic field distributions of axisymmetric micro-objects (e.g., cylinders, spheres, and spheroids) with complex refractive index ($n = n + ik$) and characteristic size a . The electromagnetic fields inside and on the surface of the microparticles can be enhanced at specific values of the size parameter $x = 2(\pi a)/\lambda$ (where λ is the optical wavelength). For dielectric microparticles, even with $x < 1$, localized surface plasmon resonances can occur at several wavelengths with vastly different electromagnetic field enhancement factors and spectral linewidths. Recent experimental interests have been directed toward the exploitation of the enhanced electromagnetic field intensity of these resonances. For dielectric microparticles in particular, morphology-dependent resonances have been applied to the determination of the following properties of individual droplets flowing in a linear stream: (a) evaporation and condensation rates; (b) interfacial surface tension and bulk viscosity; and (c) nonlinear optical properties such as lasing and coherent Raman processes. For metallic microparticles, localized surface plasmon resonances have been applied to the species determination of molecular adsorbates via the surface enhanced Raman scattering. In this presentation, research results from collaborative work at Yale, Cornell, and Clarkson Universities will be briefly reviewed.

501,467
PB85-206365 (Order as PB85-206324, PC A13/MF A01)
National Bureau of Standards, Gaithersburg, MD.
Characterization of Optical Materials and Surfaces Using Time-Domain Reflectometry.
A. G. Lieberman. Apr 85, 4p
Included in OM85: Basic Properties of Optical Materials. Summaries of Papers, p17-20 Apr 85.

Keywords: *Optical materials, Optical measurement, Light pulses, Surfaces, *Time domain reflectometry, Laser radiation, Femtosecond pulses.

The generation of femtosecond duration laser pulses containing only a few oscillations of coherent light has recently been achieved using pulse compression techniques. Such ultrashort pulses have broad spectral bandwidths which may encompass the material and structural resonances of a reflecting medium. The effects of these resonances of a reflecting medium. The effects of these resonances upon the reflected waveform could provide a novel method for characterizing the optical properties of a material or evaluating the surface finish of a manufactured object. The purpose of this paper is to explore the features of time-dependent optical pulse scattering from dispersive materials having smooth surfaces, from perfect conductors having randomly rough surfaces, and from materials exhibiting both dispersion and surface roughness.

501,468
PB85-206373 (Order as PB85-206324, PC A13/MF A01)
Naval Weapons Center, China Lake, CA.
Theory of Light Scattering from a Rough Surface with a Nonlocal Inhomogeneous Dielectric Permittivity.
J. M. Elson. Apr 85, 3p
Included in OM85: Basic Properties of Optical Materials. Summaries of Papers, p21-23 Apr 85.

Keywords: *Light scattering, *Surface roughness, Perturbation theory.

First-order perturbation theory can be used to predict the combined effect of surface roughness and dielectric inhomogeneities on the scattering of light from optical surfaces. Problems that arise, are discussed.

501,469
PB85-206381 (Order as PB85-206324, PC A13/MF A01)
Iowa State Univ., Ames.
Optical Properties of Metals in the Infrared - The Drude Model, Problems with It, and Non-Local Optics.
D. W. Lynch. Apr 85, 4p
Included in OM85: Basic Properties of Optical Materials. Summaries of Papers, p24-27 Apr 85.

Keywords: *Optical properties, *Infrared radiation, *Metals, Electron gas, *Drude model.

The infrared optical properties of metals are frequently described by a free-electron gas model, the Drude model. The author discusses several situations for which the Drude model is known not to be valid, despite its use in the literature.

501,470
PB85-206399 (Order as PB85-206324, PC A13/MF A01)
Argonne National Lab., IL.
Separation of Drude and Band-to-Band Spectra in Polyvalent Metals.
D. Y. Smith, and B. Segall. Apr 85, 4p
Prepared in cooperation with Case Western Reserve Univ., Cleveland, OH.
Included in OM85: Basic Properties of Optical Materials. Summaries of Papers, p28-31 Apr 85.

Keywords: *Optical properties, *Metals, Aluminum, Drude model.

The problem of separating intra- and interband contributions to optical properties has been reexamined with the goal of minimizing the dependence of the separation on specific models. This was prompted by a desire to compare the recently published theoretical interband spectrum of aluminum with reflectance measurements. Unfortunately, such a comparison is complicated because intra- and interband effects are almost inextricably intermeshed in the data. Several prior analy-

Field 20—PHYSICS

Group 20F—Optics

ses have been involved restrictive assumptions regarding the interband component. However, the authors present here an approach that uses general qualitative features of the theory combined with experimental data over a wide energy range that reduces the assumptions required and yields a more reliable separation.

501,471
PB85-206407

(Order as PB85-206324, PC A13/MF A01)
Naval Weapons Center, China Lake, CA.
Status of Materials for Transmissive and Reflective Infrared Components,
H. E. Bennett. Apr 85, 4p
Included in OM85: Basic Properties of Optical Materials. Summaries of Papers, p32-35 Apr 85.

Keywords: *Infrared optical materials, Absorption spectra, Zinc sulfides, Zinc selenides, Potassium chloride, Yttrium oxides, Reviews, Calcium lanthanum sulfides.

In addition to optical absorption, various other parameters must be considered in selecting an infrared transmitting material for a given application. In many cases, fracture toughness, resistance to thermal shock, and insensitivity to environmental agents such as water are of great importance.

501,472
PB85-206415

(Order as PB85-206324, PC A13/MF A01)
Wolfe Loeb and Co., Hinsdale, IL.
Dimensional Stability,
W. Primak. Apr 85, 4p
Included in OM85: Basic Properties of Optical Materials. Summaries of Papers, p36-39 Apr 85.

Keywords: *Optical materials, *Optical equipment, *Dimensional stability.

No abstract available.

501,473
PB85-206423

(Order as PB85-206324, PC A13/MF A01)
GTE Labs., Inc., Waltham, MA.
Nonlinear Optical Properties of Organic Polymer Materials,
G. M. Carter, Y. J. Chen, M. F. Rubner, M. K. Thakur, and S. K. Tripathy. Apr 85, 6p
Included in OM85: Basic Properties of Optical Materials. Summaries of Papers, p40-45 Apr 85.

Keywords: *Optical materials, *Polymers, Thin films, Molecular structure, Excitation, Raman spectroscopy, Molecular energy levels, *Polydiacetylenes, *Nonlinear optics.

Research into the nonlinear optical properties of organic polymers including such phenomena, as harmonic generation, Raman scattering, difference frequency generation, and the Kerr effect as well as including a wide variety of materials (available through organic synthesis) in various forms (e.g. solution, liquid crystal, and solid). The polydiacetylenes are an interesting nonlinear optical materials system, and current research is addressing the interrelation between their structural and the time dependent excited state properties to provide a knowledge base for potential applications. Yet the polydiacetylenes are just one interesting class of organic nonlinear optical materials. The present investigation of the nonlinearities in the PDA's can clearly set the broad direction for the investigation of other molecularly engineered organic systems for practical exploitation.

501,474
PB85-206431

(Order as PB85-206324, PC A13/MF A01)
IBM Research Lab., San Jose, CA.
Preparation of Organic Nonlinear Optical Materials for Second Harmonic Generation,
C. W. Dirk, R. J. Twieg, and G. Wagniere. Apr 85, 4p
Prepared in cooperation with Zurich Univ. (Switzerland). Inst. of Physical Chemistry.
Included in OM85: Basic Properties of Optical Materials. Summaries of Papers, p46-49 Apr 85.

Keywords: *Polymers, *Organic compounds, *Crystal structure, *Nonlinear optics, *Second harmonic generation.

No abstract available.

501,475
PB85-206449

(Order as PB85-206324, PC A13/MF A01)
Johns Hopkins Univ., Laurel, MD. Applied Physics Lab.
Optical Phase Transitions in Organo-Metallic Compounds,
T. O. Poehler, and R. S. Potember. Apr 85, 4p
Included in OM85: Basic Properties of Optical Materials. Summaries of Papers, p50-53 Apr 85.

Keywords: *Electrooptics, *Semiconducting films, *Metal containing organic compounds, Thin films, Phase transformations, Raman spectra, Complex compounds, *Optical switches, Cyclohexadiene diylidene dimalononitrile.

The authors have recently reported optical and optoelectronic switching between two states in polycrystalline organo-metallic semiconductor films using the 488.0 and 457.9 nm lines of an argon ion laser. They have now demonstrated that defocused laser radiation can be used as a source of thermal energy to reverse or erase switched regions of the film. The wavelength dependence of the optical switching threshold for CuTCNQ and AgTCNQ was studied to obtain information about the switching mechanism. Work in progress has also involved a variety of thin films of semiconducting charge-transfer complexes different from the typical AgTCNQ and CuTCNQ for which many of the previous results have been reported. Other salts which are members of the class are those formed of metal donor atoms and the organic acceptor molecule such as TCNE, TCNQ, methyl TCNQ, and TNAP.

501,476
PB85-206472

(Order as PB85-206324, PC A13/MF A01)
Toledo Univ., OH.
Optical Constants and Harmonic Generation by Surface Plasmons,
H. J. Simon. Apr 85, 5p
Included in OM85: Basic Properties of Optical Materials. Summaries of Papers, p60-64 Apr 85.

Keywords: *Optical properties, Metal films, Metals, Dielectrics, Interfaces, *Second harmonic generation, *Plasmons.

The recent prediction of the properties of a new long range surface plasmon (LRSP) mode on the two surfaces of a thin metal film bounded by index-matched dielectrics has stimulated theoretical and experimental interest in this new mode. When the fundamental mode of this plasmon is excited on both surfaces of a thin silver film bounded by a nonlinear quartz crystal and an index-matched liquid, the second harmonic generation is over two orders of magnitude larger than that due to the single-boundary surface plasmon. In conclusion, the highly resonant and localized nature of the LRSP mode will make this mode a useful new probe for studying linear and nonlinear optical properties of metal-dielectric interfaces.

501,477
PB85-206480

(Order as PB85-206324, PC A13/MF A01)
Cincinnati Univ., OH. Dept. of Electrical and Computer Engineering.
Low Loss Thin Film Materials for Integrated Optics,
H. E. Jackson, and J. T. Boyd. Apr 85, 6p
Included in OM85: Basic Properties of Optical Materials. Summaries of Papers, 65-70 Apr 85.

Keywords: Thin films, Glass, Zinc oxides, Silicon nitrides, Niobium oxides, Tantalum oxides, *Integrated optics, *Optical waveguides, Laser annealing.

The authors have reviewed their recent efforts to obtain low loss planar waveguides for potential use in integrated optics. Employing both novel fabrication and laser annealing techniques, they have achieved values of waveguide attenuation substantially below 1 dB/cm for a variety of waveguide materials. In several cases, values below 0.1 dB/cm were achieved, with efforts to achieve even lower values of waveguides attenuation continuing.

501,478
PB85-206506

(Order as PB85-206324, PC A13/MF A01)
Arizona Univ., Tucson. Optical Sciences Center.
Relationship of Microstructure to Optical Properties of Thin Films,
H. A. Macleod. Apr 85, 6p
Included in OM85: Basic Properties of Optical Materials. Summaries of Papers, p74-79 Apr 85.

Keywords: *Dielectric films, *Optical properties, *Microstructure, *Thin films, Titanium oxides, Zirconium oxides.

Although the properties of materials in thin-film form are broadly similar to those of bulk materials, there are often significant differences. Frequently the level of performance that can be achieved with thin films is inferior to that predicted from simple bulk properties. Great progress has been made in closing the gap between real thin-film properties and bulk properties but a gap still remains and much of it is a direct consequence of the effects of microstructure on the optical, mechanical and chemical properties of thin films. Here we are concerned solely with the optical properties and we limit the discussion to dielectric films.

501,479
PB85-206514

(Order as PB85-206324, PC A13/MF A01)
Royal Signals and Radar Establishment, Malvern (England).
Microstructure and Optical Properties of Thin Films Prepared by Molecular Beam Techniques,
K. L. Lewis, A. M. Pitt, J. A. Savage, A. G. Cullis, and N. G. Chew. Apr 85, 4p
Included in OM85: Basic Properties of Optical Materials. Summaries of Papers, p80-83 Apr 85.

Keywords: *Thin films, *Optical coatings, *Microstructure, Radiation damage, Optical properties, *Molecular beam epitaxy, Laser radiation.

The present work assesses the potential of molecular beam techniques for the deposition of improved optical coatings. This growth technique allows a high degree of control over the deposition process and in situ assessment techniques such as Auger and XPS allow the characterization of the surfaces produced. By combining Knudsen evaporation with RF sputtering processes in a dedicated UHV facility, it is possible to fabricate coating structures containing a wide range of different materials including sulphides, selenides, tellurides, arsenides, phosphides, fluorides, chlorides, oxides and nitrides without necessarily having to break vacuum and risk the creation of contaminated interfaces.

501,480
PB85-206522

(Order as PB85-206324, PC A13/MF A01)
Centre National de la Recherche Scientifique, Marseille (France).
Simple Model of Inhomogeneity in Optical Thin Films,
G. Deniau, F. Flory, and E. Pelletier. Apr 85, 2p
Included in OM85: Basic Properties of Optical Materials. Summaries of Papers, p84-85 Apr 85.

Keywords: *Optical coatings, *Thin films, Titanium oxides, Homogeneity, Models, Inhomogeneity.

Most materials used in thin-film optical coatings exhibit optical inhomogeneity that is frequently so large that it cannot be neglected. The inhomogeneity is directly related to the layer microstructure that can be observed in electron micrographs. This leads directly to the consideration of a layer model that can be used to represent this homogeneity and can be used in calculations. Its usefulness decreases with its complexity and it should therefore be as simple as possible but nevertheless it should also reflect the real behavior of the films. The unprecedented precision with which multilayer deposition can now be controlled coupled with the possibility of accurate in situ property measurement makes the time ripe for a reexamination of this problem.

501,481
PB85-206530

(Order as PB85-206324, PC A13/MF A01)
Optical Properties of Diamondlike Carbon Films on Semiconductors,
G. B. Bu-Abbud, J. D. Lamb, J. E. Oh, and J. A. Woollam. Apr 85, 3p
Prepared in cooperation with Universal Energy Systems, Dayton, OH.
Included in OM85: Basic Properties of Optical Materials. Summaries of Papers, p86-88 Apr 85.

Keywords: *Optical coatings, *Carbon, Optical properties, Semiconductors (Materials), Substrates, Films, Diamonds, Ellipsometry, Refractive index, Extinction coefficients.

Diamondlike carbon (DLC) films have been described by various authors as being hard, resistant to various chemicals, highly insulating, and adherent to a wide variety of materials. The authors have recently been investigating the usefulness of these materials in various applications including dielectrics for integrated circuits and coatings for optical (especially infrared) materials. The purpose of the present paper is to describe the optical properties of DLC films deposited on several technologically important semiconductors. Specifically, the authors have used spectroscopic ellipsometry and absorption spectroscopy to determine the index of refraction and extinction coefficient over the wavelength range from 220 nm to 3.39 micrometers. Substrate materials include flat, polished, oriented single crystals of silicon, indium phosphide, cadmium telluride, mercury cadmium telluride, germanium, and quartz.

501,482
PB85-206548

(Order as PB85-206324, PC A13/MF A01)
IIT Research Inst., Chicago, IL.
Temperature Dependent Optical Properties of Silver Sulfide Thin Films,
R. L. Burton, H. Buhay, M. Nisar, J. L. Grieser, and N. P. Murarka. Apr 85, 4p
Included in OM85: Basic Properties of Optical Materials. Summaries of Papers, p89-92 Apr 85.

Keywords: *Silver sulfides, *Infrared optical materials, Thin films, Refractive index, Extinction coefficients.

Flash evaporation techniques for synthesizing Ag₂S thin films have been reported elsewhere. In this work, results are presented for films prepared by a triode D.C. sputtering process which has been found to provide greater control and produced superior films. Optical transmittance and reflectance measurements were made using a Perkin-Elmer Model 580B spectrophotometer. From the optical data, the frequency dependence of the refractive index n and extinction coefficient k were computed.

501,483
PB85-206555

(Order as PB85-206324, PC A13/MF A01)
Colorado State Univ., Fort Collins. Dept. of Physics.
Molecular Bonding in Optical Films Deposited by Ion-Beam Sputtering,
C. Y. She. Apr 85, 6p
Included in OM85: Basic Properties of Optical Materials. Summaries of Papers, p93-98 Apr 85.

Keywords: *Optical coatings, *Titanium dioxide, *Molecular structure, Crystal structure, Raman spectroscopy, Sputtering, Films, Laser annealing.

Using Raman spectroscopy, we have studied the microscopic structure and molecular bonding of ion-beam sputtered optical films by the method of thermal and laser annealing. Transformation of amorphous titanium coatings to crystalline anatase and/or rutile structures has been observed. We report these results and discuss their implications in this paper.

501,484
PB85-206563

(Order as PB85-206324, PC A13/MF A01)
Bell Communications Research, Inc., Murray Hill, NJ.
Highly Transparent Metal Films: Pt ON InP,
D. E. Aspnes, A. Heller, J. D. Porter, T. T. Sheng, and R. G. Vadimsky. Apr 85, 4p
Prepared in cooperation with Bell Labs., Murray Hill, NJ.
Included in OM85: Basic Properties of Optical Materials. Summaries of Papers, p99-102 Apr 85.

Keywords: *Metal films, *Platinum, *Optical coatings, *Transparency, Indium phosphides.

Highly transparent metal films are of potential interest in a number of areas of science and technology including light detection, photovoltaic energy conversion, catalysis, and photoelectrochemistry. In studies of light-activated photocatalysis on platinized semiconducting photocathodes, it was discovered that the quantum yield of hydrogen-evolving semiconducting electrodes did not decline significantly with increasing platinum coverages, even for metric thicknesses as much as 50 nm where 99.9% of the transmitted light should have been absorbed. The observation of this anomalous transparency stimulated further investigation, and in a recent preliminary report the authors described the preparation and characterization of the first substantially transparent supported metal films of sig-

nificant thicknesses. They found that the essential characteristics giving rise to substantial transparency in metal films were porosity and microstructure, and that by controlling these properties, absorption and reflection losses could almost be eliminated. Here, the authors discuss in more detail the physical principles involved and present further results on Pt film/p-InP system.

501,485
PB85-206571

(Order as PB85-206324, PC A13/MF A01)
Pennsylvania Univ., Philadelphia.
Calculation of the Electronic Structure of As₄S₄ and As₄Se₄ Molecules,
D. Babic, and S. Rabii. Apr 85, 3p
Included in OM85: Basic Properties of Optical Materials. Summaries of Papers, p103-105 Apr 85.

Keywords: *Molecular structure, Molecular energy levels, Ionization potentials, *Arsenic sulfides, *Arsenic selenides, *Electronic structure, Integrated optics, Amorphous materials.

The recent developments in preparation of thin amorphous films of the arsenic chalcogenides by spin-coating from solution have led to renewed interest in these materials for applications in the field of integrated optics as waveguides, couplers, or storage media. As part of our theoretical investigation of the electronic structure of these materials, we have undertaken to calculate the molecular structure for some of their existing molecules, namely As₄S₄, As₄Se₄, As₄S₆ and As₄Se₆. In the present paper we report on our calculations for the first two molecules.

501,486
PB85-206589

(Order as PB85-206324, PC A13/MF A01)
IIT Research Inst., Chicago, IL.
Free-Carrier Absorption in a Thin Film Silver Sulfide Galvanic Cell,
R. L. Burton, H. Buhay, J. L. Grieser, and N. P. Murarka. Apr 85, 4p
Included in OM85: Basic Properties of Optical Materials. Summaries of Papers, p106-109 Apr 85.

Keywords: Silver sulfides, *Infrared optical materials, *Electrolytic cells, Thin films, Transmittance, Reflectance, Refractive index, Extinction coefficients.

Ag₂S undergoes a crystallographic phase transition at a temperature $T_c = 180^\circ\text{C}$. The electrical conductivity of the high temperature phase, $\alpha\text{-Ag}_2\text{S}$, is three orders of magnitude greater than the low temperature phase, $\beta\text{-Ag}_2\text{S}$. As a result, $\beta\text{-Ag}_2\text{S}$ transmits through much of the mid-infrared region, whereas $\alpha\text{-Ag}_2\text{S}$ exhibits a distinct plasma absorption edge. Studies of the influence of the electron concentration on the electrical and optical properties of bulk Ag₂S have been reported. Investigations of these properties were achieved by incorporating an AgS sample in a galvanic cell structure. The structure of these bulk material galvanic cells is given by: Ag electrode/AgI/Ag₂S/Pt electrode. In a similar manner a thin film galvanic cell, with a design analogous to the bulk cell, has been made and used to vary the electron concentration in the silver sulfide film of the cell. Several thin film silver sulfide galvanic cells were prepared. The transmittance and reflectance data are shown. The corresponding refractive index and extinction coefficient computed from the best fit parameters are shown. Also given is a plot of electron concentration as a function of cell potential.

501,487
PB85-206597

(Order as PB85-206324, PC A13/MF A01)
Naval Weapons Center, China Lake, CA.
Synthesis and Characterization of Stoichiometric CdPS₃,
J. Covino, P. Dragovich, and C. Lowe-Ma. Apr 85, 5p
Included in OM85: Basic Properties of Optical Materials. Summaries of Papers, p110-114 Apr 85.

Keywords: *Infrared optical materials, *Synthesis(Chemistry), X ray diffraction, Selenides, Sulfides, *Cadmium phosphide sulfides, Cadmium phosphide selenide sulfides.

CdPS₃ is optically transparent from 4000/cm to 500/cm (2.5-20 micrometers) with a fundamental absorption edge close to 454/cm (22 micrometers). Initial studies of CdPS₃ suggested that the material could be useful as an infrared transmitting material provided that the material strength could be increased. CdPS₃

has been synthesized with stoichiometry much closer to the theoretical value previously reported. The present X-ray data for the CdPS₃ system, although reproducible from sample to sample, is not consistent with the C₂/m structure assigned to this compound by Brec et al. However, the presently reported data are consistent with a layer structure in which cadmium might be in a different environment or in more than one environment. If cadmium is in a second environment then it must be, as the (113)Cd NMR shows, only one Cd(II) site. Furthermore, as seen by the EPR data of Mn-doped CdPS₃ this cadmium site whether it be interstitial or defect cannot be substituted by Mn(II). Such structural differences could also explain the different intercalation chemistries of the cadmium and nickel MPS₃ compounds.

501,488
PB85-206605

(Order as PB85-206324, PC A13/MF A01)
Energy Conversion Devices, Inc., Troy, MI.
Characterization of Thin Semiconducting Films on Transparent Substrates,
B. Edgerton, and D. Shortt. Apr 85, 4p
Included in OM85: Basic Properties of Optical Materials. Summaries of Papers, p115-118 Apr 85.

Keywords: *Semiconducting films, Thin films, Glass, Transparency, Substrates, Amorphous silicon, Refractive index, Extinction coefficients.

Uniform homogenous layers of material deposited on a substrate can be described optically by a thickness and a complex index of refraction, $n(\lambda) - ik(\lambda)$. Alternately one can describe the absorption coefficient, $\alpha(E)$, as a function of the photon energy. If the complex index of refraction and the thickness are known for both the film and the substrate, then electromagnetic theory provides a basis for calculating the reflectance and transmittance spectra of the film. The challenge is to work this problem backwards. Given the two spectra, can one find a unique description of the dispersion in the optical properties as well as a thickness which satisfy the data. The first step in our process is to choose a parameterized model to describe the optical properties. The second part of the process determines the values of the optical properties without recourse to a particular choice of parameterized model for describing the shape of the dispersion. The film used to illustrate this technique is a glow discharge deposition of amorphous silicon hydrogen alloy on Corning 7059 glass. The measured spectra appear in Fig. 1.

501,489
PB85-206613

(Order as PB85-206324, PC A13/MF A01)
Alexandria Univ. (Egypt). Faculty of Engineering.
Laser Propagation through Fibers with Biquadratic Refractive Index (Closed Form Solution),
F. Z. El-Halafawy, A. Y. Rezk, and E. A. Al-Badawy. Apr 85, 3p
Included in OM85: Basic Properties of Optical Materials. Summaries of Papers, p119-121 Apr 85.

Keywords: *Laser beams, *Light transmission, *Fiber optics, *Mathematical models, Intensity, *Optical fibers.

In this paper, closed form equations for both trajectories and intensity profiles of a light beam traveling in a continuous media of biquadratic graded refractive index are derived avoiding the approximations made by other authors. In conclusion, biquadratic-index media yields self-trapping if its parameters and the launch conditions are adjusted.

501,490
PB85-206621

(Order as PB85-206324, PC A13/MF A01)
National Bureau of Standards, Gaithersburg, MD. Inorganic Materials Div.
Densification of Zirconia Films by Coevaporation with Silica,
A. Feldman, and E. N. Farabaugh. Apr 85, 4p
Included in OM85: Basic Properties of Optical Materials. Summaries of Papers, p122-125 Apr 85.

Keywords: *Optical coatings, *Zirconium oxides, *Silicon dioxide, Electron beams, Substrates, Films, Coevaporation, Refractive index.

Optical films of zirconia have been receiving considerable attention because of their potential use as the high-index layer in multilayer optical coatings for the

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ultraviolet portion of the spectrum. Several problems are associated with electron-beam deposited zirconia films and these include index instability and index inhomogeneity. The index instability is caused by the adsorption and the desorption of water in the porous columnar structure of the zirconia films. Index inhomogeneity is due to the inhomogeneous structure in the films. Recent work has shown that the first several tens of nanometers of a film possess a cubic structure whereas the outmost layers possess a monoclinic structure. One approach for producing bulk-like zirconia films that is receiving considerable attention at present is ion-assisted electron-beam deposition. This is because the method has successfully produced zirconia films having bulk-like densities and refractive indices that show insignificant sensitivity to water adsorption. In this paper we demonstrate a similar effect when mixed zirconia:silica films are produced by coevaporation from independent electron-beam sources, and, in particular, we show that the admixture of a small amount of silica with the zirconia produces a film possessing a higher refractive index than a pure zirconia film.

501,491
PB85-206639

(Order as PB85-206324, PC A13/MF A01)
Massachusetts Inst. of Tech., Cambridge.

Temperature Dependence of the VUV (Vacuum Ultraviolet) Optical Spectra and Band Structure of Al₂O₃

R. H. French, and R. L. Coble. Apr 85, 4p
Included in OM85: Basic Properties of Optical Materials. Summaries of Papers, p126-129 Apr 85.

Keywords: *Aluminum oxide, *Band structure of solids, *Energy bands, Far ultraviolet radiation, Ultraviolet spectra, Single crystals, Reflectivity, High temperature tests, *Electronic structure, Temperature dependence.

A high temperature vacuum ultraviolet (VUV) spectrophotometer has been built that is capable of measuring the reflectance and transmittance of samples from 6 eV to 15 eV (210 nm to 85 nm) in the VUV on samples heated without contamination from room temperature up to 1100C. The precision (reproducibility) of the measurements is 0.01 eV, the resolution of the monochromator is 0.1 eV while the spectrophotometer can resolve 0.3 eV wide spectral features of the sample. The temperature dependence of the electronic structure of single crystal Al₂O₃ has been studied with this facility.

501,492
PB85-206654

(Order as PB85-206324, PC A13/MF A01)
Naval Weapons Center, China Lake, CA.

EPR (Electron Paramagnetic Resonance) Studies of Infrared-Transmitting Sulfide Ceramics

D. C. Harris, M. E. Hills, J. Covino, C. K. Lowe-Ma, and R. W. Schwartz. Apr 85, 4p
Included in OM85: Basic Properties of Optical Materials. Summaries of Papers, p133-136 Apr 85.

Keywords: *Infrared optical materials, Optical properties, Crystal defects, Impurities, *Calcium lanthanum sulfides, *Aluminum zinc sulfides, Electron spin resonance.

Calcium lanthanum sulfide (nominally CaLa₂S₄) and zinc aluminum sulfide (ZnAl₂S₄) are potentially useful as infrared-transmitting ceramics. In an attempt to correlate optical properties with the presence of impurities and defects, the authors have been studying the electron paramagnetic resonance (EPR) spectra of powdered samples. EPR spectroscopy has established that CaS is an impurity phase in CaLa₂S₄ and has been used to identify transition metal impurities, paramagnetic defects and photochemical processes in these materials. Both Mn(2+) and a paramagnetic center with coupling to several (27)Al nuclei were observed in preparation of ZnAl₂S₄. These spectra may be useful in evaluating the quality of ZnAl₂S₄ preparations and in the identification of impurity phases that are present.

501,493
PB85-206662

(Order as PB85-206324, PC A13/MF A01)
Raytheon Co., Lexington, MA. Research Div.

Elastic Properties of Chemically Vapor-Deposited ZnS and ZnSe

C. A. Klein, and C. B. Willingham. Apr 85, 4p
Included in OM85: Basic Properties of Optical Materials. Summaries of Papers, p137-140 Apr 85.

Keywords: *Zinc selenides, *Zinc sulfides, *Elastic properties, Waveguide windows, Infrared windows, Chemical vapor deposition.

Material characteristics such as Young's modulus and Poisson's ratio play an important role in designing optical windows or assessing their performance from the point of view of thermally-induced distortion as well as pressure-induced fracture. The elastic properties of interest in the study include Young's modulus, the shear modulus, the bulk modulus, Poisson's ratio, the velocity of compressional waves, and the velocity of shear waves.

501,494
PB85-206670

(Order as PB85-206324, PC A13/MF A01)
Litton Systems, Inc., Woodland Hills, CA. Guidance and Control Systems Div.

Radiation Effects in a Glass-Ceramic (Zerodur)

N. Koumvakalis, M. G. Jani, and L. E. Halliburton. Apr 85, 4p
Prepared in cooperation with Oklahoma State Univ., Stillwater, Dept. of Physics.
Included in OM85: Basic Properties of Optical Materials. Summaries of Papers, p141-144 Apr 85.

Keywords: *Optical materials, *Radiation effects, *Ceramic composites, Gyroscopes, Quartz, Ionizing radiation, *Zerodur, Laser gyroscopes.

Zerodur is a low-expansion glass-ceramic with important applications in laser-gyro guidance systems. The material contains by weight 70-75% crystalline quartz in the form of crystallites approximately 50 nm in diameter which are embedded in a glass matrix. The glass-crystal ratio is adjusted so that the resultant expansion coefficient at room temperature is near zero. Ionizing radiation causes numerous effects in Zerodur. The most obvious is a change in the optical absorption, and this will have possible consequences in the thermal expansion behavior. Thus, characterization of radiation-induced defects will help solve problems affecting Zerodur's performance in guidance systems and will provide an understanding of the basic properties of this unique class of materials.

501,495
PB85-206720

(Order as PB85-206324, PC A13/MF A01)
Concordia Univ., Sir George Williams Campus, Montreal (Quebec). Dept. of Electrical Engineering.

Properties of Guided Modes in Bidirectional Anisotropic Media

O. Schwelb. Apr 85, 4p
Included in OM85: Basic Properties of Optical Materials. Summaries of Papers, p160-163 Apr 85.

Keywords: *Light transmission, Matrices(Mathematics), Transfer functions, Optical waveguides.

Explicit expression have been presented for the layer transfer matrix, for the characteristic impedance and for the bounds of the effective guide index for uniaxial media in polar and longitudinal orientation. Some properties distinguishing the equatorial orientation have also been mentioned.

501,496
PB85-206738

(Order as PB85-206324, PC A13/MF A01)
University of Southern California, Los Angeles. Center for Laser Studies.

Calorimetric Measurement of Optical Absorption in Sapphire at Visible, near IR, and near UV Wavelengths

A. B. Villaverde, R. T. Swimm, and M. Bass. Apr 85, 3p
Included in OM85: Basic Properties of Optical Materials. Summaries of Papers, p164-166 Apr 85.

Keywords: *Sapphire, Near infrared radiation, Near ultraviolet radiation, Single crystals, *Absorption coefficients, Laser radiation.

The optical absorption of sapphire was measured calorimetrically in the wavelength interval from 1.32 micrometer to 0.35 micrometer. The data show reasonably linear behavior in a plot of the natural logarithm of the absorption due to residual chromium ions.

501,497
PB85-206761

(Order as PB85-206324, PC A13/MF A01)
Naval Research Lab., Washington, DC.

Status of Optical Constants of Solids from X-ray to MM-Wave Region

E. D. Palik. Apr 85, 6p
Included in OM85: Basic Properties of Optical Materials. Summaries of Papers, p171-176 Apr 85.

Keywords: X rays, Ultraviolet radiation, Light(Visible radiation), Infrared radiation, Millimeter waves, Thin films, *Refractive index, *Extinction coefficients.

As editor of the Handbook of Optical Constants of Solids (1) the author has obtained a bird's-eye view of the quantity and quality of optical constants for 37 solids of technological and physics interest. These include 11 metals - Al, Cu, Au, Ir, Mo, Ni, Os, Pt, Rh, Ag, W; 14 semiconductors - CdTe, GaAs, GaP, Ge, InAs, InSb, InP, PbSe, PbS, PbTe, Si, a-Si, ZnS; 12 insulators - As₂Se₃, As₂S₃ (diamond), LiF, LiNbO₃, KCl, SiO₂, SiO, Si₃N₄, NaCl, TiO₂. Twenty one critiquers have examined the existing literature for these materials and have tabulated a single set of refractive index *n* and extinction coefficient *k* for as wide a spectral region as possible. Examples of a metal Ag, a semiconductor Si and an insulator a-SiO₂ (silica) are given in Fig. 1. Some effort is made to discuss the measurement techniques and the quality of the data. The problems encountered here with measurements and data are representative. The problems encountered here with measurements and data are representative of all the solids studied. The Handbook also contains 11 chapters on how to determine *n* and *k* in various spectral regions.

501,498
PB85-206779

(Order as PB85-206324, PC A13/MF A01)
Argonne National Lab., IL.

Optical Constants at X-ray Wavelengths

D. Y. Smith, A. E. Williamson, and T. I. Morrison. Apr 85, 4p
Included in OM85: Basic Properties of Optical Materials. Summaries of Papers, p177-180 Apr 85.

Keywords: *X ray absorption, Absorption spectra, Synchrotron radiation.

The present paper is a preliminary report on optical properties of selected elements at x-ray wavelengths as derived from measured absorption spectra. Need for such data is an outgrowth of the world-wide development of synchrotron radiation sources: the reflectance is of interest for designing grazing-incidence mirrors, and knowledge of optical constants is required to calculate the properties of multilayer elements, as well as to analyze differential absorption and anomalous scattering experiments.

501,499
PB85-206787

(Order as PB85-206324, PC A13/MF A01)
Bell Labs., Holmdel, NJ.

Vacuum Ultraviolet Loss in Magnesium Fluoride Films

O. R. Wood, P. J. Maloney, H. G. Craighead, and J. E. Sweeney. Apr 85, 3p
Included in OM85: Basic Properties of Optical Materials. Summaries of Papers, p181-183 Apr 85.

Keywords: *Optical costs, *Magnesium fluoride, *Far ultraviolet radiation, *Ultraviolet optical materials, Light scattering, Losses, Thin films.

Because MgF₂ is transparent to wavelengths as short as 1100 Å in the VUV, it finds extensive use for lenses and windows in this region. Major applications can be found in UV lasers, spectroscopy and space astronomy. Another important use of MgF₂ is as an evaporated coating onto aluminum, where it greatly increases the VUV reflectance and also retards oxidation. The authors have investigated the excess loss in evaporated films and found that it is due to scattering from inhomogeneities and absorption from the low energy tail of an excitation band. Both of these mechanisms were found to be strongly dependent on the degree of crystallinity of the film, which is largely determined by the substrate temperature during deposition. The study has allowed the authors to produce films with extinction coefficients as low as 0.005, several times better than previously reported.

501,500
PB85-206829

(Order as PB85-206324, PC A13/MF A01)
Princeton Univ., NJ.

Micro-Raman Study of Laser-Induced Damage,
P. M. Fauchet, I. H. Campbell, and F. Adar. Apr 85, 4p
Prepared in cooperation with Instruments S.A., Inc., Metuchen, NJ.
Included in OM85: Basic Properties of Optical Materials. Summaries of Papers, p198-201 Apr 85.

Keywords: *Radiation damage, *Raman spectroscopy, Optical materials, *Laser radiation, Neodymium lasers.

In most laser systems, damage to optical components is the major factor that limits scaling towards higher energy density. Although laser-induced damage in solids has been an active field of research for many years the authors do not have a satisfactory understanding of the physics involved in these processes. This situation is in part due to the lack of nondestructive, quantitative probes that can be used in situ. In this paper, the authors show that Raman scattering is such a probe and can be used successfully in a wide range of practical situations.

501,501
PB85-206837
(Order as PB85-206324, PC A13/MF A01)
Bell Labs., Holmdel, NJ.
Optical Effects in Quantum Well Structures and Superlattices,
D. S. Chemla. Apr 85, 12p
Included in OM85: Basic Properties of Optical Materials. Summaries of Papers, p202-213 Apr 85.

Keywords: Gallium arsenides, *Quantum wells, Superlattices, Aluminum gallium arsenides, Nonlinear optics.

The author has presented some recent progress made in the investigation and the utilization of the excitonic resonances observed at room temperature in GaAs/AlGaAs multiple quantum well structures. Novel nonlinear optical and electro-optical effects are observed which result from the lowered dimensionality of the electrons in ultra-thin semiconductor layers. Room temperature excitonic peak are not only interesting for the applications, they also exhibit the most unusual properties owing to their extremely short life time and their transformation into free e-h pairs.

501,502
PB85-206845
(Order as PB85-206324, PC A13/MF A01)
Naval Research Lab., Washington, DC.
Photorefractance in GaAs/AlGaAs Multiple Quantum Wells,
O. J. Glembocki, B. V. Shanabrook, N. Bottka, W. T. Beard, and J. Comas. Apr 85, 4p
Included in OM85: Basic Properties of Optical Materials. Summaries of Papers, p214-217 Apr 85.

Keywords: Gallium arsenides, *Quantum wells, *Photorefractance, Aluminum gallium arsenides, Heterojunctions.

Recently, the authors demonstrated that photorefractance is a sensitive probe of interband transitions in GaAs/Al(x)Ga(1-x)As multiple quantum wells (MQW) and modulation doped heterojunctions exhibiting a two dimensional electron gas. In this paper, the authors describe the photorefractance technique and review the results of the MQW work found in another paper.

501,503
PB85-206860
(Order as PB85-206324, PC A13/MF A01)
Eidgenössische Technische Hochschule, Zurich (Switzerland).
Photorefractive and Nonlinear-Optical Properties of New Electrooptic Materials,
P. Günter. Apr 85, 4p
Included in OM85: Basic Properties of Optical Materials. Summaries of Papers, p222-225 Apr 85.

Keywords: *Electrooptics, Optical materials, Signal processing, Organic compounds, Reviews, Photorefractive effect, Nonlinear optics.

In this paper, the author presents a review of both photorefractive and nonlinear-optical materials for optoelectronic applications. The materials requirements for nonlinear optical laser frequency conversion using the electronic hyper-polarizabilities and optical signal processing using the photorefractive and nonlinear optical materials, its properties and applications are described.

501,504
PB85-206878
(Order as PB85-206324, PC A13/MF A01)
Hughes Research Labs., Malibu, CA.
Measurement of Defect and Transport Properties of Electro-Optic Materials Using the Photorefractive Effect,
M. B. Klein, and G. C. Valley. Apr 85, 3p
Included in OM85: Basic Properties of Optical Materials. Summaries of Papers, p226-228 Apr 85.

Keywords: *Electrooptics, Optical materials, Optical measurement, Transport properties, Barium titanates, *Photorefractive effect, Sodium barium niobates, Barium strontium niobates.

In this paper, the authors use steady state beam coupling as a function of grating period at 442 nm to obtain data on the sign of the dominant photocarrier, the concentration of empty traps and the effective electro-optic coefficient for several samples of BaTiO₃, Ba₂NaNb₅O₁₅ (BNN) and Sr(1-x)Ba(x)Nb₂O₆ (SBN). The authors assume an energy level model in which a single species X, in two valence states XX and X(+), is responsible for the photoactive energy states in the bandgap of each sample. The authors denote the concentration of X as N, and that of X(+) as N(+). The authors allow for the photo-generation of both electrons and holes, through the ionization of X or X(+), respectively.

501,505
PB85-206886
(Order as PB85-206324, PC A13/MF A01)
Oklahoma State Univ., Stillwater.
Analysis of Scattering Patterns and Decay Dynamics of Photorefractive Gratings in LiNbO₃ Crystals,
J. K. Tymiński, R. C. Powell, H. C. Chow, and M. J. Kleiwer. Apr 85, 3p
Included in OM85: Basic Properties of Optical Materials. Summaries of Papers, p229-231 Apr 85.

Keywords: *Gratings(Spectra), Laser beams, Single crystals, Holography, Crystal defects, Light scattering, *Lithium niobates, *Photorefractive effect.

One technique for studying the photorefractive effect (PRE) in crystals is to establish and probe holographic gratings with crossed laser beams. Generally the gratings are assumed to have a sinusoidal shape and the measurement which is made is the scattering efficiency of the probe beam at the Bragg condition. The authors report the development of a new technique for studying the PRE based on the analysis of small angle scattering patterns. This technique allows for the inclusion of multiple fourier components in the geometric shape of the grating in analysis to LiNbO₃ crystals with several different types of defect properties show that the measured scattering patterns are extremely sensitive to the microscopic properties of the grating.

501,506
PB85-206894
(Order as PB85-206324, PC A13/MF A01)
University of Southern California, Los Angeles.
Use of Optical Phase Conjugation for Understanding Basic Material Properties,
R. W. Hellwarth. Apr 85, 2p
Included in OM85: Basic Properties of Optical Materials. Summaries of Papers, p232-233 Apr 85.

Keywords: Barium titanates, *Phase conjugation, Four wave mixing, Photorefractive effect, Bismuth silicates, Semiconductors.

In the simplest class of phase-conjugation experiments the two beams E and G interfere to create intensity variations (moving or stationary) which in turn cause a variation in the refractive index seen by beam H. This variation is often called an index 'grating'. The H beam scatters from this grating to generate the F beam. This may be called the (tensor) volume holographic process for phase-conjugation. The beams can be on simultaneously or in various time sequences. The authors will describe how this single-grating process has been used to obtain the most accurate measurements of impurity density, conduction band diffusion lengths, and trap excitation cross-sections in photorefractive bismuth silicate and barium titanate. Results for electron-hole pairs in semiconductors will also be described. This process gives often the simplest and most accurate method of measuring thermal conductivities of slightly absorbing transparent media. It is also the basis for another coherent Raman spectroscopic technique (Raman-induced phase con-

jugation) which has advantages and disadvantages relative to coherent anti-Stokes Raman spectroscopy and other well-known laser spectroscopic techniques.

501,507
PB85-206910
(Order as PB85-206324, PC A13/MF A01)
Hughes Research Labs., Malibu, CA.
Refractive Indices and Thermo-Optic Coefficients of Nonlinear Crystals Isomorphous to KH₂PO₄,
K. W. Kirby, C. S. Hofer, and L. G. DeShazer. Apr 85, 4p
Included in OM85: Basic Properties of Optical Materials. Summaries of Papers, p238-241 Apr 85.

Keywords: Light(Visible radiation), Near infrared radiation, Ammonium compounds, Cesium inorganic compounds, Rubidium compounds, Potassium inorganic compounds, Deuterium compounds, Arsenates, Thermal properties, Electrooptics, *Potassium hydrogen phosphates, *Refractive index, Phosphates, Nonlinear optics.

Crystals of the potassium dihydrogen phosphate (KDP) group are widely used in laser technology. These tetragonal isomorphs have the composition MH₂XO₄, where M may be K, Rb, Cs or NH₄; X may be P or As; and H may be replaced by deuterium D, fully or partly. They encompass sixteen crystals potentially useful in state-of-the-art optical devices. These devices are second harmonic generators, sum and difference frequency mixers, electro-optical switches, and phase modulators. The refractive indices and their thermal behavior were measured for eleven of these nonlinear crystals (table 1). These parameters are needed to establish the phase matching geometry and thermal behavior of a nonlinear crystal in the frequency upconversion operation in high-power laser systems.

501,508
PB85-206928
(Order as PB85-206324, PC A13/MF A01)
San Jose State Univ., CA.
Bismuth Silicon Oxide: Sample Variability Studied with Thermally Stimulated Conductivity and Thermoluminescence,
B. W. Holmes, and J. E. Ludman. Apr 85, 4p
Prepared in cooperation with Rome Air Development Center, Hanscom AFB, MA.
Included in OM85: Basic Properties of Optical Materials. Summaries of Papers, p242-245 Apr 85.

Keywords: *Thermoluminescence, Variability, Electron traps, Holography, *Bismuth silicon oxides, Photorefractive effect, Phase conjugation.

Bismuth silicon oxide (BSO) is widely used in optical data processing, reversible, real-time holography, and optical phase conjugation. The optical characteristics (such as wavefront reflectivity) vary significantly, even for identically prepared crystals. The manufacture of uniform and improved BSO crystals may well depend on a better understanding of the fundamental processes responsible for its photosensitivity. The authors studied electron trapping in BSO using thermally stimulated conductivity (TSC) and thermoluminescence (TL). In this study, the authors surveyed at a number of different BSO crystals, in order to assess sample variability as revealed in TSC and TL.

501,509
PB85-206936
(Order as PB85-206324, PC A13/MF A01)
Arizona Univ., Tucson. Optical Sciences Center.
Materials Requirements for Optical Logic and Bistable Devices,
N. Peyghambarian, and H. M. Gibbs. Apr 85, 3p
Included in OM85: Basic Properties of Optical Materials. Summaries of Papers, p246-248 Apr 85.

Keywords: Gates(Circuits), Zinc sulfides, Zinc selenides, Gallium arsenides, *Optical bistability, *Logic devices, Nonlinear optics, Refractive index, Aluminum gallium arsenides, Copper chlorides, Semiconductors.

Optical bistability, which is referred to as the existence of two stable output intensities for the same input intensity, has been realized in many semiconductors. Examples include the GaAs and GaAs-AlGaAs multiple-quantum-well superlattices, CuCl, and ZnSe. In this talk, the authors focus their attention on these materials because of their greater potential to be used as practical devices.

Field 20—PHYSICS

Group 20F—Optics

501,510

PB85-206944

(Order as PB85-206324, PC A13/MF A01)
Rensselaer Polytechnic Inst., Troy, NY.

Mirrorless Optical Bistability in CdS,

J. W. Haus, C. C. Sung, C. M. Bowden, and J. M.

Cook. Apr 85, 2p

Prepared in cooperation with Alabama Univ. in Huntsville. Dept. of Physics, Army Missile Command, Redstone Arsenal, AL., and Middle Tennessee State Univ., Murfreesboro.

Included in OM85: Basic Properties of Optical Materials. Summaries of Papers, p249-250 Apr 85.

Keywords: *Cadmium sulfides, *Optical bistability, Logic devices.

Recently, Dagenais and Sharfin have reported whole-beam optically bistable behavior in uncoated platelets of CdS. This phenomenon was observed at milliwatt power levels when the incident laser frequency was tuned just below the resonance of the $I(2)$ bound-excitation. Using a qualitative model, the authors successfully correlated the temperature dependence of the absorption with the observed bistable behavior. The authors research extends their qualitative model by eliminating several unnecessary assumptions. It is shown how such devices can be used as multiplexers and as composite optical logic elements and for use in optical computing and optical communications. The role of the temperature-induced absorption in CdS which leads to bistable output intensities is explained.

501,511

PB85-206951

(Order as PB85-206324, PC A13/MF A01)

Lockheed Missiles and Space Co., Inc., Palo Alto, CA.

Nonlinear Optical Effects in Liquid Crystals,

D. Armitage, and S. M. Delwart. Apr 85, 4p

Included in OM85: Basic Properties of Optical Materials. Summaries of Papers, p251-254 Apr 85.

Keywords: *Liquid crystals, Birefringence, Nonlinear optics.

Liquid crystals are birefringent materials with fluidity comparable to water. Device potential arises from the influence of electric, magnetic or optic fields on the optic axis orientation. The response time is viscous limited. However, the more viscous smectic phases have storage properties. The birefringence is directly related to the order parameter of the fluid and its therefore sensitive to temperature, particularly near a phase transition. As the nematic to isotropic phase transition, the refractive index (n) discontinuity approximates 0.1. This is a weak first order transition with latent heat approximately 1 J/cc. These properties make the nematic phase an interesting solvent in a thermal dye cell. The thermal response is not viscous limited. It can be shown that when submillisecond response is demanded the thermal process is more efficient than the viscous limited orientation response. Experiments were performed with 5CB doped with L-dye D81 (EM Chemicals).

501,512

PB85-206969

(Order as PB85-206324, PC A13/MF A01)

Anhui Inst. of Optics and Fine Mechanics (China).

Study of Second Harmonic Generation Coefficients and Ultraviolet Absorption Edge of Barium Borate Crystal,

J. K. Zhu, B. Zhang, and S. H. Liu. Apr 85, 1p

Included in OM85: Basic Properties of Optical Materials. Summaries of Papers, p255 Apr 85.

Keywords: Ultraviolet radiation, Wave functions, *Barium borates, *Second harmonic generation, Nonlinear optics.

Barium borate (β -BaB₂O₄) is a new type of nonlinear optical crystal. In this paper the authors report one-electron energies and wave functions of barium borate by use of EMO theory. Both the calculated values of SHG coefficient and ultraviolet absorption edge for barium borate crystal are in quantitative agreement with the experimental results. The comparison between EMO, CNDO/S and experimental values is shown.

501,513

PB85-206977

(Order as PB85-206324, PC A13/MF A01)

Alexandria Univ. (Egypt).

Soliton Transmission in Inhomogeneous Media with W-Tailored Refractive Index,

F. A. El-Halafawy, E. A. El-Badawy, M. A. El-

Gammal, and M. H. Aly. Apr 85, 4p

Included in OM85: Basic Properties of Optical Materials. Summaries of Papers, p256-259 Apr 85.

Keywords: *Fiber optics, *Optical fibers, *Solitons, Refractive index.

In this paper, a method for soliton transmission in inhomogeneous media with W-tailored refractive index is modeled and parametrically analyzed. Two kinds of inhomogeneities are simultaneously considered: (a) Biquadratic variation of the refractive index (W-tailored radial profile), and (b) Boundary conditions of the clad-fiber.

501,514

PB85-206985

(Order as PB85-206324, PC A13/MF A01)

BDM Corp., Albuquerque, NM.

Comparison of Vibrational Spectra of Heavy Metal Fluoride Glasses with Those of 'Common' Glasses,

B. Bendow. Apr 85, 6p

Included in OM85: Basic Properties of Optical Materials. Summaries of Papers, p260-265 Apr 85.

Keywords: *Vibrational spectra, *Glasses, *Optical glass, *Fluorides, *Infrared optical materials, Infrared spectra, Raman spectra, Chemical bonds, Molecular structure, Devitrified glass, Comparison, Heavy metals.

Vibrational spectroscopy, including polarized Raman scattering and fundamental IR reflectivity (Reststrahlen spectra), has been used to study the structure and bonding of many glasses, and to determine the origins of observed IR edge characteristics. In this paper, the authors reviews the spectra obtained to date for heavy metal fluoride glasses, and compares them with the spectra of simple halide, oxide and chalcogenide glasses.

501,515

PB85-206993

(Order as PB85-206324, PC A13/MF A01)

Schott Glaswerke, Mainz (Germany, F.R.).

Verdet Constant of Optical Glasses,

H. J. Hoffmann, W. W. Jochs, and G. Przybilla. Apr

85, 4p

Included in OM85: Basic Properties of Optical Materials. Summaries of Papers, p266-269 Apr 85.

Keywords: *Optical glass, *Glass, *Faraday effect, *Magnetooptics, *Verdet constants, Polarized light.

A relation for the Verdet constant as a function of wavelength was first derived by Becquerel. Unfortunately Becquerel's equation cannot generally be justified on the basis of quantum mechanics. L. Rosenfeld calculated a quantum mechanical expression of the Faraday rotation angle for the monoatomic case. A thorough discussion of the limitations is given by Van Vleck. In order to avoid these difficulties, the authors developed recently a simple new dispersion formula. To test this equation, they determined experimentally the Verdet constant of different glasses in the visible spectral region by measuring the rotation angle induced by a magnetic field.

501,516

PB85-207009

(Order as PB85-206324, PC A13/MF A01)

National Defense Academy, Yokosuka (Japan).

Temperature Dependence of Magneto-optic Effects in Mid-Infrared Fibers,

H. Sato, Y. Azumai, and M. Saito. Apr 85, 4p

Prepared in cooperation with Horiba Ltd., Kyoto (Japan). Research and Development Dept.

Included in OM85: Basic Properties of Optical Materials. Summaries of Papers, p270-273 Apr 85.

Keywords: *Infrared optical materials, *Magnetooptics, *Faraday effect, *Fiber optics, Intermediate infrared radiation, *Optical fibers, Temperature dependence, Verdet constants, Arsenic sulfides.

In the present paper, low temperature properties of KRS-5 and As₂S₃ fibers are described about their magneto-optic effects such as the Faraday- and Voigt effects at CO₂ 10.6 micrometer and He-Ne 3.39 micrometer laser radiation.

501,517

PB85-207017

(Order as PB85-206324, PC A13/MF A01)

GTE Labs., Inc., Waltham, MA.

Optical Characterization of Devitrification for Cr(+3)-Doped Zr-Ba-La-Al Fluoride Glass,

W. J. Miniscalco, L. J. Andrews, B. T. Hall, and D. E.

Guenther. Apr 85, 4p

Included in OM85: Basic Properties of Optical Materials. Summaries of Papers, p274-277 Apr 85.

Keywords: *Devitrified glass, *Optical glass, *Fluorides, Infrared optical materials, Atomic energy levels, Emission spectroscopy, Photoluminescence, Chromium, Stability, Crystal field, Doped materials, Heavy metals.

The past decade has seen an enormous increase in activity in the area of heavy metal fluoride glasses. These glasses contain no oxygen and are distinguished from the fluoroberyllates by the absence of beryllium. In addition to their scientific interest as a largely unexplored glass-forming system, heavy metal fluoride glasses are of technological interest because they have high optical transmission from the UV to the mid-IR (\approx or $>$ 7 micrometers). One potential application is as optical fiber for both communications and energy transmission in the mid-IR. Since these glasses can be doped with transition metal and rare earth ions, other promising applications are as solid state laser hosts and magneto-optic devices. An important consideration in all applications is the relatively poor stability of these glasses compared to oxide glasses as indicated by their extremely narrow working ranges. Even for the best compositions the crystallization temperature is seldom more than 100 degrees C higher than the glass transition temperature. To further understand the stability of heavy metal fluoride glasses, the authors have undertaken an investigation of crystallization using primarily optical techniques. The work has concentrated on a Zr-Ba-La-Al fluorozirconate glass (ZBLA) which has been doped with probe ions whose optical spectra are sensitive to their local environment.

501,518

PB85-207025

(Order as PB85-206324, PC A13/MF A01)

Israel Atomic Energy Commission, Yavne. Soreq Nuclear Research Center.

Optical Study of Ge-P-Te and Ge-Se-Te Chalcogenide Glasses,

L. Boehm, A. Bornstein, and S. Arie. Apr 85, 4p

Included in OM85: Basic Properties of Optical Materials. Summaries of Papers, p278-281 Apr 85.

Keywords: *Infrared optical materials, *Fiber optics, Group 6A compounds, Chemical analysis, X ray analysis, Chemical composition, Optical properties, *Germanium phosphide tellurides, *Germanium selenide tellurides, *Optical fibers.

Chalcogenide glasses have been thoroughly investigated, especially in connection with their electronic properties and their promise as IR windows in the 8-12 micrometers region. For the purpose of the present study, the major attraction of chalcogenides lies in their promise as IR materials for infrared optical fibers. Such fibers are needed in applications using high-power CO₂ laser for surgery as well as in cutting and heat treatment of metals. These fibers will also play an important role in the development of many infrared devices in the field of image relaying and remote sensing. In this study, the authors present the preparation and optical characterization of two glass systems containing relatively high amounts of Te. Such glasses are expected to be transparent up to 20 micrometer and may serve as preforms for drawing IR fibers.

501,519

PB85-207256

Not available NTIS

National Bureau of Standards (NML), Boulder, CO.

Quantum Physics Div.

Precision Measurements by Optical Heterodyne Techniques,

Final rept.,

L. Hollberg, M. Long-Sheng, M. Hohenstatt, and J. L.

Hall. 1984, 8p

Contract NSF-PHY82-00805

Pub. in Proceedings of SPIE - The International Society for Optical Engineering, San Diego, CA., August 23-24, 1983, p91-98 1984.

Keywords: *Optical measurement, *Heterodyning, Iodine, Line spectra, Erbium, Absorption spectra, Spectroscopy, Four wave mixing.

Optical heterodyne techniques are described that are generally applicable to spectroscopy and precision measurements. Phase modulation is used at high fre-

quencies in order to suppress laser amplitude noise which is dominantly at low frequencies. The high sensitivity of these techniques is demonstrated in the detection of non-linear optical resonances in molecular iodine. Optical heterodyne saturated absorption and four-wave-mixing spectra taken with a dye laser are shown of the 612 nm I₂ line which is of importance for optical frequency standards. Also shown are optical heterodyne detected saturated absorption spectra of Erbium taken in a hollow cathode discharge. An improvement in signal-to-noise ratio of 1000 is found for the optical heterodyne method relative to optogalvanic signals detected in the same discharge. Advantages and disadvantages of the various methods are discussed as are some ideas for improvement. A list of thirty references is given.

501,520
PB85-207355 Not available NTIS
National Bureau of Standards (NEL), Boulder, CO.
Electromagnetic Technology Div.
Using Optical Processing to Find the Beam Profile of a Laser Pulse (Theory).
Final rept.,
E. G. Johnson. 1984, 14p
Pub. in Proceedings of SPIE--Optical Radiation Measurements 499, p75-88 1984.

Keywords: *Laser beams, Light pulses, Cross correlation, Reprints, *Beam profiles, Optical processing.

The paper looks at a particular form of optical processing, namely a form of cross-correlation, and demonstrates how the method measures certain beam profile features of a laser pulse. Beam profile is defined to mean a description of the electromagnetic field of a laser pulse in space and time.

501,521
PB85-208114 Not available NTIS
National Bureau of Standards (NML), Boulder, CO.
Time and Frequency Div.
Optical Frequency Synthesis Spectroscopy.
Final rept.,
K. M. Evenson, D. A. Jennings, F. R. Petersen, J. S. Wells, and R. E. Drullinger. 1984, 9p
Pub. in Progress in Quantum Electron 8, p143-151 1984.

Keywords: *Frequency measurement, *Electron transitions, Iodine, Reprints, Visible radiation, State of the art.

In order to measure the super narrow spectral features of cooled atoms and ions, in the optical region, optical frequency synthesis (OFS) techniques rather than wavelength techniques must be used. It is anticipated that many of these resonances will be in the optical region of the spectrum, and this paper addresses the state-of-the-art of the measurements of frequencies in that region. Two recent optical frequency measurements of iodine transitions in the visible are described, as well as recent improvements in fabricating the point-contact diode used in these measurements.

501,522
PB85-208122 Not available NTIS
National Bureau of Standards (NEL), Boulder, CO.
Electromagnetic Technology Div.
Attenuation of Multimode Fused Silica Optical Fibers Cooled to Liquid Helium Temperature.
Final rept.,
A. Engelsrath, D. R. Larson, D. L. Franzen, and R. J. Phelan. 1984, 7p
Pub. in Proceedings of SPIE -- Fiber Optics: Short-Haul and Long-Haul Measurements and Applications II, n500 p124-130 1984.

Keywords: Fiber optics, Attenuation, Near infrared radiation, Detectors, Silicon dioxide, Cryogenics, *Optical fibers, Visible radiation, Multimode.

The feasibility of bringing an optical signal through an optical fiber to a detection and processing system at liquid helium temperature was examined. The attenuation of three multimode optical fibers, from two different manufacturers with different buffer coatings, was measured under different cooling conditions. It was found that the attenuation depends on the cooling condition and has hysteresis effects. Independent of the wavelength tested (0.4 - 1.65 micrometers) the attenuation stayed below 0.1 dB/m under controlled slow cooling and under 0.5 dB/m with very fast cooling. Therefore, optical fibers can be used to bring optical signals into a liquid helium cooled Dewar for detection and processing.

501,523
PB85-222008 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Laser Wavelength Meters.
Final rept.,
J. J. Snyder. 1982, 7p
Pub. in Laser Focus 18, n5 p55-61 1982.

Keywords: *Wavelengths, Measuring instruments, Optical interferometers, Reviews, Measurement, Metrology, Reprints, *Laser radiation.

A review of devices that may provide routine and rapid measurements with high accuracy and resolution.

501,524
PB85-229268 Not available NTIS
National Bureau of Standards (NML), Boulder, CO.
Quantum Physics Div.
Theory of Resonant Degenerate Four-Wave Mixing with Broad-Bandwidth Lasers.
Final rept.,
G. Alber, J. Cooper, and P. Ewart. 1985, 1p
Grant NSF-PHY82-00805
Pub. in Physical Review A 31, n4 p2344-2352 Apr 85.

Keywords: Laser beams, Band width, Reprints, *Four wave mixing, *Degenerate four wave mixing, Nonlinear optics.

The effects of finite laser bandwidth on resonant degenerate four-wave mixing (DFWM) are calculated with use of a model in which the intense, counter-propagating pump beams are characterized by a chaotic field, the probe beam is weak and monochromatic, and the medium consists of a gas of two-level atoms. The authors present a steady-state solution in the limit where the pump-laser bandwidth exceeds all other atomic relaxation rates. Although the mean intensity due to the fluctuating fields is spatially independent (no steady-state standing-wave pattern is established), the analytic results indicate that, for intensities above the saturation intensity $I(\text{sat})$, spatially periodic saturation effects are important. Increasing bandwidth is shown to lead to an increase in the effective saturation intensity resulting in lower phase-conjugate reflectivity for $I < I(\text{sat})$ than for coherent pump fields, in contrast to the results for narrow-bandwidth chaotic fields. The resonant DFWM line shape is also calculated and compared to the coherent result. The authors comment on the application of the model to other four-wave-mixing processes employing broad-bandwidth lasers.

501,525
PB86-122785 Not available NTIS
National Bureau of Standards (NML), Boulder, CO.
Quantum Physics Div.
Coherent Raman Spectroscopy.
Final rept.,
M. D. Levenson, and J. J. Song. 1980, 80p
Pub. in Coherent Nonlinear Optics Recent Advances, p293-372 1980.

Keywords: *Raman spectroscopy, Reviews, *Coherent antistokes raman spectroscopy, Four wave mixing, Nonlinear optics.

A comprehensive review is given of work on coherent Raman spectroscopy including sections on history, theory, experimental techniques, and applications. An extensive bibliography of more than 200 entries is included.

501,526
PB86-124054 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD.
Atomic and Plasma Radiation Div.
Grazing-Incidence High-Resolution Stigmatic Spectrograph with Two Optical Elements.
Final rept.,
A. M. Malvezzi, L. Garifo, and G. Tondello. 1981, 6p
Pub. in Applied Optics 20, n14 p2560-2565, 15 Jul 81.

Keywords: *Ultraviolet spectrometers, *Spectrographs, Reprints, *Ultraviolet telescopes, *Solar spectrometers.

Using two optical toroidal elements, a mirror and a grating, both working at grazing incidence, a spectrometer can be built that is stigmatic in the XUV region at one wavelength. Good compensation of the aberrations is achieved when the intermediate sagittal image is nearly at infinity. By varying the angle of incidence on the grating with simple movements, a given couple

of optical elements could cover stigmatically a rather extended spectral range. If coupled with bidimensional array detectors, such a spectrograph could find applications in planned solar XUV telescopes.

501,527
PB86-132743 PC A04/MF A01
National Bureau of Standards (NEL), Boulder, CO.
Electromagnetic Technology Div.
Direct Measurement of the Electric Field of a Laser Pulse - Theory.
Technical note,
E. G. Johnson. Aug 85, 60p NBS/TN-1084
Also available from Supt. of Docs as SN003-003-02697-2.

Keywords: *Laser beams, *Electric fields, Light pulses, Measurement, Fiber optics, Optical filters, Beam profiles.

The author considers realizing an electric field measuring apparatus by using optical processing, tapered optical fibers, and a pair of detectors at the end of each optical fiber. Using an appropriate computer-generated optical filter, the author shows it is possible to discriminate among a set of orthonormal modes used to represent the spatial features of the electric field with a signal-to-noise ratio of at least 100 to 1. If the positioning accuracies for various parts of the apparatus are properly set up, it is expected that the signal-to-noise ratio could be about 1000. The purpose of the tapered and graded-index fiber is to select the fundamental propagating mode in a fiber and to attenuate the other modes. The existence of this fiber allows the precise determination of the strength of each of the orthonormal modes being used as the spatial basis of the electric field before the optical processing. The paper presents the conflicts in the design and gives a solution. The complete evaluation requires assembly of the proposed apparatus to assess final accuracy.

501,528
PB86-138013 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Inorganic Materials Div.
Determination of Fringe Order in the Channel Spectra of Thin-Films.
Final rept.,
A. Feldman. 1984, 4p
Pub. in Applied Optics 23, n8 p1193-1196 1984.

Keywords: *Optical interference, *Thin films, Optical coatings, Thickness, Reprints, Refractive index, Dispersion.

The fringe orders in the channel spectrum of a thin film can be determined unambiguously provided it is known that the film thickness is less than a critical value. The value is equal to minus one half the reciprocal dispersion of the material at the wavelength of minimum dispersion within the wavelength range of measurement. Values of critical thickness are given, as a function of wavelength, for 33 optical materials. The data indicate that the critical thickness is at least 10 micrometers in all of the materials at wavelengths within the operating range of commercial spectrophotometers.

501,529
PB86-139805 Not available NTIS
National Bureau of Standards (NEL), Boulder, CO.
Electromagnetic Technology Div.
Some Issues In Optical Fiber Bandwidth Measurements.
Final rept.,
S. Yang, and R. L. Gallawa. 1985, 1p
Pub. in IEEE Instrumentation and Measurement Technology Conference, Tampa, FL., March 20-22, 1985, p228.

Keywords: *Fiber optics, *Bandwidth, Measurement, *Optical fibers.

This is a one-page summary of a talk given at the IEEE Instrumentation and Measurement Technology Conference. The talk discusses the measurement of optical fiber bandwidth, using methods in common use in the fiber community. Difficulties and variabilities are discussed.

501,530
PB86-140308 Not available NTIS
National Bureau of Standards (NEL), Boulder, CO.
Electromagnetic Technology Div.

Field 20—PHYSICS

Group 20F—Optics

Some Trends In Optical Electronic Metrology.

Final rept.,
A. A. Sanders. 1984, 7p
Pub. in Proceedings of the Measurement Science Conference (1984), Long Beach, California, January 19-20, 1984, p27-33.

Keywords: *Fiber optics, *Electrooptics, *Metrology, *Optical fibers, Integrated optics, Laser applications, US NBS.

The use of optical related devices in high technology is expanding at a dramatic rate. Applications include the expanding use of optical fibers in telecommunications and sensors, lasers in industrial processing and medicine, optical storage devices, directed energy weapons for defensive purposes, non-destructive testing, etc. The Optical Electronics Metrology Group of the National Bureau of Standards has the responsibility for developing the standards, measurement data and methodology infrastructure for supporting much of this expanding technology. The paper reviews some of the ongoing research currently conducted by this group, and some of the perceived important technological applications in this area for the next few years. It discusses Group plans for developing the measurement infrastructure to support these innovations.

501,531

PB86-142387 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Building Physics Div.
Visual Clarity with a Black-and-White Scene.
Final rept.,
J. A. Worthey. 1985, 5p
See also AD-A141 498.
Pub. in Jnl. of the Illuminating Engineering Society 14, n2 p634-647 Apr 85.

Keywords: *Visual perception, Color vision, Experiments, Recognition, Resolution, Visual acuity, Reprints.

Visual clarity experiments are usually done with colorful test objects, and it is generally concluded that the results of such experiments are related to the color-rendering properties of the illuminants involved. Nonetheless, it has been observed that a clarity difference between illuminants may be seen, even with black-and-white objects. An experiment was performed to measure differences of perceived clarity using only black-and-white fabric and black yarn as test objects. (The word 'clarity' was not used in the instructions to subjects. They were asked questions concerning 'preferences' and 'blackness'.) The differences measured seem to indicate a role for color in black-and-white vision, but not a pure clarity effect independent of illuminant color.

501,532

PB86-142395 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Building Physics Div.
Limitations of Color Constancy.
Final rept.,
J. A. Worthey. 1985, 13p
Pub. in Jnl. of the Optical Society of America A2, n7 p1014-1026 Jul 85.

Keywords: *Color, *Adaptation, Visual perception, Chroma, Illuminance, Reprints.

Theories of adaptation, such as those based on the proportionality law of von Kries, provide detailed predictions concerning perception of object colors when illuminant spectral power distribution is changed. Since these predictions depart from the simple ideal of color constancy, a question arises of the relationships among data, theories, and the ideal of constancy. Projecting the data of a constancy experiment into an opponent-color system indicates that constancy tends to hold well for illuminant shifts in the blue-yellow direction but less well for shifts in the red-green direction. This observation is consistent with a theory based on von Kries adaptation.

501,533

PB86-142825 Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div.
Bandwidth of a Multimode Fiber Chain.
Final rept.,
P. M. Rodhe. Feb 85, 10p
Pub. in Jnl. of Lightwave Technology LT-3, n1 p145-154, 1 Feb 85.

Keywords: *Fiber optics, *Bandwidth, Transfer functions, Optical measurement, Reprints, *Optical fibers, Multimode.

The author proposes a new method for evaluating the baseband transmission in a multimode fiber chain. Carnevale and Paek stated that errors in the fiber manufacturing process will randomly distort a desired index profile, presumably of power-law type. The author extends their discussion to the band-widths of concatenated fibers, by considering Gaussian approximations to actual transfer functions. The bandwidth can thus be separated into two parts, one of which is due to the over- and undercompensation of individual, idealized power-law profiles, and the other of which refers to random profile distortions as well as possible mode coupling within mode groups.

501,534

PB86-142833 Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div.
Intramodal Part of the Transfer Function for an Optical Fiber.
Final rept.,
P. M. Rodhe. Feb 85, 5p
Pub. in Jnl. of Lightwave Technology LT-3, n1 p154-158, 1 Feb 85.

Keywords: *Fiber optics, *Transfer functions, *Bandwidth, Optical measurement, Reprints, *Optical fibers.

Intramodal contributions in measurements of optical-fiber bandwidth are investigated theoretically and experimentally in the quasimonochromatic case. A relation is established between the intramodal transfer function and a possibly non-Gaussian source spectrum, which may also vary with modulation frequency. By considering the latter variation in particular, we are able to predict the intramodal length dependence and show how it may deviate from that of a conventional approach.

20G. Particle Accelerators

501,535

PB86-112372 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Source and Instrumentation Div.
Note on the Lawson-Penner Limit.
Final rept.,
J. D. Lawson, and S. Penner. Feb 85, 1p
Pub. in IEEE (Institute of Electrical and Electronics Engineers) Jnl. of Quantum Electronics QE-21, n2 p174 Feb 85.

Keywords: Electron accelerators, Linear accelerators, Reprints, *Lawson-Penner limit, Free electron lasers.

No abstract available.

20H. Particle Physics

501,536

PB85-172211 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Experimental Test of the Bremsstrahlung Cross Section.
Final rept.,
M. N. Martins, E. Hayward, G. Lamaze, X. K. Maruyama, and F. Shima. Dec 84, 6p
Pub. in Physical Review C 30, n6 p1855-1860 Dec 84.

Keywords: Bremsstrahlung, Cross sections, Electron beams, Gamma rays, Reprints, *Bremsstrahlung cross sections, Electrodintegration, Copper 63, MeV range 10-100, Photon-neutron interactions.

The bremsstrahlung cross section has been studied by measuring the activity induced in (63)Cu by electrodintegration and when thin radiators of Cu, Mo, Ta, and Th were placed in the electron beam just ahead of the target. The electron energies were varied from 13.5 to 60 MeV for the electrodintegration and from 20 to 60 MeV for the radiator-in measurements; the (gamma,n) cross section for (63)Cu was determined using virtual photon theory; the radiator data were fitted using various bremsstrahlung cross sections. The best fit is ob-

tained using the synthesized spectrum of Seltzer which differs from the Davies-Bethe-Maximon cross section as given by equation (3CS) of Koch and Motz.

501,537

PB85-189454 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Standardization of Technetium-99 by Liquid-Scintillation Counting.
Final rept.,
B. M. Coursey, J. A. B. Gibson, M. W. Heitzmann, and J. C. Leak. 1984, 10p
Pub. in International Jnl. of Applied Radiation and Isotopes 35, n12 p1103-1112 1984.

Keywords: Standardization, Beta decay, Half life, Gravimetric analysis, Reprints, *Technetium 99, Liquid scintillators.

Technetium-99 has been standardized by comparing its pulse-height response on a liquid-scintillation counter with that of another beta-particle-emitting standard radionuclide. In this work, hydrogen-3, carbon-14, and cobalt-60 were used as the standards, and the results obtained agreed to within 0.32%. The mass of potassium pertechnetate was also measured by gravimetric techniques for the technetium-99 radioactivity standard solution. A half-life value of $(2.111 \pm 0.012) \times 10^5$ to the 5th power years is suggested. The estimated uncertainty is intended to approximate one standard deviation.

501,538

PB85-189462 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Nuclear Radiation Div.
Coincidence Form Factors in Electron Scattering.
Final rept.,
J. S. O'Connell. 1984, 21p
Grant NSF-PHY84-09410
Sponsored by Connecticut Univ. Research Foundation, Storrs.
Pub. in Proceedings of Workshop of the Bates Users Theory Group (3rd), Massachusetts Institute of Technology, Cambridge, MA, July 23-24, 1984, p1-21.

Keywords: *Electron scattering, Inelastic scattering, Quarks, Pions, Form factors, Nuclear resonance.

The two-body breakup cross section of inelastic electron scattering is presented and discussed. Examples of model calculations and some data are given for resonances, direct reactions, pion production, and scattering from quarks.

501,539

PB85-203503 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Cascade Effects in Mass-Dependent Preferential Recoil Implantation.
Final rept.,
M. L. Roush, F. Davarya, O. F. Goktepe, and T. D. Andreadis. 1983, 12p
Pub. in Nuclear Instruments and Methods in Physics Research 209, p67-78 May 83.

Keywords: Computerized simulation, Reprints, *Ion bombardment, Ion implantation, Recoils.

Under some circumstances, ion bombardment induces preferential recoil implantation of one species of an initially homogeneous binary target. The atomic masses of the target components play a central role in the segregation produced by the ion bombardment if all binding energies are the same. The process of component segregation does not generally take place by single recoil implantation events in which atoms are driven from the surface region inward to the enriched portion. Rather, the motion is one of migration in which a great deal of motion takes place due to atomic mixing and there is a slight directional preference which favors the inward movement of the heavy element. To facilitate a study of their role in recoil implantation, this computer simulation involves grouping of the components of the recoil cascade according to the number of collisions preceding their generation. The authors observe that the recoils of the lighter target species have greater total path lengths but their direction of travel is more random. The heavy species is preferentially implanted due to its retention of the inward-directed momentum.

501,540

PB85-222024 Not available NTIS

National Bureau of Standards (NML), Gaithersburg, MD. Nuclear Radiation Div.

Possible Interpretation of a New Resonance at 8.3 GeV.

Final rept., K. Lane, S. Meshkov, and F. Wilczek. 29 Oct 84, 3p. Contract EY-76-C-02-1545, Grant NSF-PHY77-27084. Sponsored by National Aeronautics and Space Administration, Washington, DC. Pub. in *Physical Review Letters* 53, n18 p1718-1720, 29 Oct 84.

Keywords: Reprints, *Pseudoscalars, Nuclear resonance, Tau particles, Gauge theory.

It is discussed whether the recently discovered resonance at 8.3 GeV can be interpreted as a weakly coupled fundamental pseudoscalar. Such a particle is readily incorporated in an SU(2) x U(1) gauge theory framework. The importance of mixing with (η sub B), (η prime sub B) for the phenomenology of such a particle is emphasized, and critical tests of their identification are proposed.

501,541
PB85-229284 Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.

New Atomic Mechanism for Positron Production in Heavy-Ion Collisions.

Final rept., W. Lichten, and A. Robatino. Feb 85, 5p. Pub. in *Physical Review Letters* 54, n8 p781-784, 25 Feb 85.

Keywords: Reprints, *Positron sources, Heavy ion reactions.

The Letter gives a newly considered mechanism for positron production which consists of filling of long-lived, supercritical, multiple-vacancy states via higher-order perturbations, with interference terms of the same order of magnitude as in the case of the previously considered single vacancies. The mechanism could be relevant to the structure in positron energy spectra observed at Gesellschaft für Schwerionenforschung in heavy-ion collisions. A possible directional anisotropy of positron emission is discussed.

501,542
PB86-103009 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Nuclear Radiation Div.

Transplutonium (σ sub nf) Systematics in the MeV Range.

Final rept., J. W. Behrens, J. Trochon, and J. Jary. Jun 85, 3p. Pub. in *Transactions of the American Nuclear Society* 49, p196-198 Jun 85.

Keywords: *Fission cross sections, *Actinide series, Reprints.

In addition to obtaining nuclear data from measurement and theory, one may also rely on nuclear data phenomenology, the study of systematic trends in nuclear parameters which are accurately known to infer these parameters for nuclides which are not accurately known, often because they are difficult to measure. One such study deals with the systematics of neutron-induced fission cross sections over the incident-neutron energy range from 1 to 20 MeV. Results for a total of over 40 isotopes of the uranians, neptuniums, and plutonians have now been completed. Extension of these trends to the transplutoniums, however, yields inferred values which significantly overpredict the fission cross section. This overprediction is primarily caused by the change in the systematics of the inner fission barrier height, near compound nucleus neutron number 146, as will be shown.

501,543
PB86-103595 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Nuclear Radiation Div.

Nuclear Data Standards.

Final rept., A. D. Carlson. 1985, 2p. Pub. in *Transactions of the American Nuclear Society* 49, p205-206 1985.

Keywords: *Neutron cross sections, *Standards, Reprints.

The rationale, need, and requirements for neutron cross section standards are discussed.

501,544
PB86-111739 Not available NTIS

National Bureau of Standards (NML), Gaithersburg, MD. Radiation Source and Instrumentation Div.

Status Report: Electro-Nuclear Physics at NBS (National Bureau of Standards).

Final rept., S. Penner. 1985, 6p. Pub. in *Proceedings of the International School of Nuclear Physics Nuclear and Subnuclear Degrees of Freedom and Lepton Nucleus Scattering*, Erice, Italy, April 8-20, 1984, *Progress in Particle and Nuclear Physics* 13, p237-242 1985.

Keywords: *Research, Electron scattering, Photonuclear reactions, Reviews, Electrodisintegration, Race-track microtrons.

Electronuclear Physics has a long history at NBS, extending back to the pioneering photonuclear experiments of Fuller and Hayward in the 1950's. Since 1967 the authors have carried out an experimental program in electron scattering, electrodisintegration, and photon scattering using their 140 MeV linac. Although there are still some experiments in progress using the linac, it is approaching the end of its useful life for nuclear physics. The authors are now building a 200 MeV CW racetrack microtron (RTM) and designing apparatus for use in a program of primarily coincidence experiments when the RTM is completed. In the report, the authors summarize the current status of these efforts, as well as experiments being carried out at other laboratories, and a small but active theory program.

501,545
PB86-114055 Not available NTIS

National Bureau of Standards (NML), Gaithersburg, MD. Nuclear Radiation Div.

Use of Electron Rings in Nuclear Physics Research.

Final rept., J. S. O'Connell. 1982, 3p. Pub. in *Proceedings of Workshop on the Use of Electron Rings for Nuclear Physics Research in the Intermediate Energy Region*, Lund, Sweden, October 5-7, 1982, v1 p1-3.

Keywords: *Electron rings.

The use of stored beams of high energy electrons for electromagnetic nuclear reactions studies is discussed in the context of the past and future of nuclear physics.

501,546
PB86-119369 Not available NTIS

National Bureau of Standards (NML), Gaithersburg, MD. Nuclear Radiation Div.

Virtual Photons in Theory and Experiment.

Final rept., W. R. Dodge. 1985, 9p. Pub. in *Nuclear Instruments and Methods in Physics Research B10/11*, p423-431 1985.

Keywords: Reprints, *Virtual photons, Virtual particles, Electrodisintegration, Zirconium 90, Isobaric analogs.

Before the last decade nuclear electrodisintegration experiments in the region of the giant dipole resonance were carried out primarily as an expedient experimental alternative to photodisintegration experiments. Lack of an adequate treatment of Coulomb distortion of the incident and scattered electron's wavefunction in heavy nuclei and recoil in light nuclei when the momentum of the scattered electron was not much smaller than the momentum of the recoiling residual nucleus limited the establishment of the correspondence between photo- and electrodisintegration to roughly s-d shell nuclei. Distorted-wave Born approximation calculations have solved the former problem in virtual photon analysis of (e,X) total cross-section measurements and the effects of recoil on PWBA virtual photons have been recently investigated. In principle, an inclusive (e,X) experiment completely determines the (γ,X) cross-section. Besides those matrix elements present in the photodisintegration cross-section that are associated with the transverse form factor as $q \rightarrow \omega$, other terms associated with the Coulomb, interference, and polarization terms of the ($e,e'X$) cross-section appear in the (e,X) cross-section. Inclusive (e,X) experiments done at NBS to test the limitations of E1 virtual photon theory are described. The proliferation of ($e,e'X$) experiments will intensify interest in ($e,e'X$) theory experiments, with the X arm singles serving as an important check on the internal consistency of the ($e,e'X$) results.

501,547
PB86-130127 Not available NTIS

National Bureau of Standards (NML), Gaithersburg, MD. Nuclear Radiation Div.

Cold Fragmentation Measurements Using a Very-High-Energy-Resolution Ionization Chamber.

Final rept., J. Trochon, G. Simon, J. W. Behrens, and F. Brisard. 1985, 1p. Pub. in *Transactions of the American Nuclear Society* 49, p199 Jun 85.

Keywords: *Nuclear fission, *Nuclear models, Thermal neutrons, Reprints, *Fission fragments, Uranium 235.

The evolution of a fissioning nucleus from saddle point to scission is perhaps the least known stage of nuclear fission at low energy. In a recent 'microscopic analysis of collective dynamics in low energy fission' using a density dependent Hartree-Fock-Bogolyubov approach with an effective force, Berger et al. interpreted the phenomenon as a passage of the nucleus from an elongation valley to a fusion valley. For small elongation, this passage occurs through a striction barrier, which disappears for more elongated configurations. This fission mode is named 'cold configuration' or 'cold fragmentation' because the scission leaves the two fragments in states close to their ground state. In the present measurements, the authors investigated cold fragmentation in the thermal neutron-induced fission of (^{235}U), i.e., ($^{236}\text{U}^*$), to test the fission dynamics calculation and to contribute to the knowledge of the even-odd effect and of the maximum total fragment kinetic energy for a given fragmentation.

501,548
PB86-139847 Not available NTIS

National Bureau of Standards (NML), Gaithersburg, MD. Nuclear Radiation Div.

Fission Cross-Section Measurements in Reactor Physics and Dosimetry Benchmarks.

Final rept., J. A. Grundl, and D. M. Gilliam. 1983, 2p. Pub. in *Transactions of the American Nuclear Society* 44, p533-535 Jun 83.

Keywords: *Fission cross sections, *Uranium 233, *Plutonium 239, *Uranium 235, Californium 252, Fission neutrons, Standards, Reprints, *Plutonium 240, *Plutonium 241, *Thorium 232, *Uranium 238, *Neptunium 237, Benchmarks.

Fission cross sections for eight fissionable isotopes of importance for nuclear technology have been measured in two fission neutron spectra and one fission-neutron-driven standard neutron field. New measurements for (^{240}Pu), (^{241}Pu), (^{233}U), and (^{232}Th), accompany revised values from earlier determinations for (^{239}Pu), (^{235}U), (^{238}U), and (^{237}Np). The starting point for all of these measurements is an absolute cross section measurement for (^{252}Cf) fission spectrum neutrons. The absolute cross section is determined from a neutron source strength, a source-to-detector distance, and an absolute fission rate. Errors are given at one standard deviation. These benchmark measurement results are intended to provide integral normalizations and a test of differential neutron cross section data.

501,549
PB86-140365 Not available NTIS

National Bureau of Standards (NML), Gaithersburg, MD. Nuclear Radiation Div.

(e,p) and (e,α) Reactions in (^{90}Zr) and (^{92}Zr).

Final rept., W. R. Dodge, E. Hayward, M. N. Martins, and E. Wolyne. Sep 85, 8p. Sponsored by Conselho Nacional de Desenvolvimento Científico e Tecnológico, Rio de Janeiro (Brazil), and National Science Foundation, Washington, DC. Pub. in *Physical Review C* 32, n3 p781-788 Sep 85.

Keywords: Alpha particle reactions, Photodisintegration, Reprints, *Zirconium 90, *Zirconium 92, Electron-proton interactions, Electrodisintegration, Virtual photons.

The yields of protons and alpha particles from 2 mg/sq cm targets of (^{90}Zr) and (^{92}Zr) have been measured in the incident electron energy range 20-100 MeV; the (^{90}Zr) (e,α) data were extended to 130 MeV. Photodisintegration plus electrodisintegration yields were also measured for electron energies above 50 MeV. The photodisintegration cross sections, derived from

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these data, rise continuously from 25 MeV onward for all four reactions. One satisfactory explanation of the phenomenon is that the authors are observing multi-particle emission following virtual photon absorption.

501,550
PB86-140373 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Office of Radiation Measurement.
Estimate of the Proton Yield from Quasi-Elastic Scattering on (sup 16)O at an Incident Electron Energy of 800 MeV.
Final rept.,
W. R. Dodge. Jul 85, 2p
Pub. in Proceedings of the Nuclear Physics with Electromagnetic Probes Europhysics Divisional Conference (11th), Paris, France, July 1-5, 1985, p248-249.

Keywords: *Protons, Electrons, Elastic scattering, Estimates, Polarized beams, Response functions, Oxygen 16.

The yield of protons from ((e vector)e'p) on 16O has been calculated using the relativistic singlet P(1/2) and singlet P(3/2) shell response functions of Van Orden et al. The total proton yield for protons with energies from 35 to 155 MeV is given as a function of the laboratory proton angle.

501,551
PB86-141934 PC A04/MF A01
National Bureau of Standards (NML), Gaithersburg, MD. Cneter for Radiation Research.
Angular Distribution of High Energy Electrons Following Radiation,
L. C. Maximon, and A. Lepretre. Oct 85, 53p NBSIR-84/2854
Prepared in cooperation with CEA Centre d'Etudes Nucleaires de Saclay, Gif-sur-Yvette (France). Service de la Metrologie et de la Physique Neutroniques Fondamentales.

Keywords: *Electron scattering, Bremsstrahlung, Scattering cross sections, Angular distribution, Screening, Small angle scattering.

An expression is derived for the angular distribution of high energy electrons which have undergone scattering and radiated a photon, integrated over the directions of the emitted photon, in the region of small scattering angles, for which the atomic form factor must be taken into account but the nuclear structure may be neglected. This distribution is analogous to Schiff's high-energy small-angle distribution for photons, integrated over the final electron angles. It is shown that the correction to the energy-angle distribution of electrons due to atomic screening is identical in form to the correction to the energy-angle distribution of photons. This correction involves an integral over the atomic form factor, and is evaluated in closed form for the Thomas-Fermi-Moliere model. A very simple expression is obtained for the case of complete screening.

20I. Plasma Physics

501,552
PB85-207413 Not available NTIS
National Bureau of Standards (NML), Boulder, CO. Quantum Physics Div.
Ionization in Gas Discharges: Experiment and Modeling.
Final rept.,
A. V. Phelps. 1985, 9p
Pub. in Electron Impact Ionization, p335-343 1985.

Keywords: *Gas discharges, *Gas ionization, Electron beams, Interactions.

The report is a brief review of electron impact ionization in gas discharges. First, the various methods of measuring ionization coefficients in gases are reviewed, with emphasis on the differences expected at high electric field E to gas density ratios. Next, theoretical calculations or models of the ionization coefficients are summarized. Finally, the role of electron impact ionization in various discharge forms are reviewed.

501,553
PB85-222040 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Atomic and Plasma Radiation Div.

Redistribution of Radiation in a Low Density Plasma.

Final rept.,
G. G. Lombardi, and D. E. Kelleher. 1983, 11p
Pub. in Proceedings of Int. Conf. Spectral Line Shapes (6th), Boulder, CO., July 12-16, 1982, v2 p835-845.

Keywords: *Hydrogen, *Fluorescence, Light scattering, Spectral lines, *Plasma, Laser radiation, Balmer lines.

The redistribution of radiation was observed in (H sub alpha), the first Balmer line of hydrogen. A dye laser was tuned to the far wing of (H sub alpha), and the fluorescent radiation was observed in the core as a function of laser detuning. The profile, which was found to be Lorentzian, is principally determined by the natural and resonance broadening of the lower level. The polarization of the fluorescent radiation was measured relative to the incident linear polarization. The polarization of the fluorescence in the absence of collisions was calculated and compared to the measured value. It provides information concerning the rate of depolarizing collisions.

501,554
PB85-229417 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Atomic and Plasma Radiation Div.
Measurement of the Ti(x)ion Density in a Theta-Pinch Plasma by a Laser Heterodyne Quadrature Interferometer.
Final rept.,
R. U. Datla. 1985, 5p
Sponsored by Department of Energy, Washington, DC. Office of Fusion Energy.
Pub. in Physical Review A 31, n4 p2764-2767 Apr 85.

Keywords: Interferometers, Impurities, Measurement, Reprints, *Plasma, *Titanium ions, *Ion density, *Electron density, Theta pinch.

The increase in the radial line integral of the electron density in the National Bureau of Standards theta-pinch plasma due to the ionization of the titanium impurity has been measured with the use of a He-Ne laser heterodyne quadrature interferometer. Titanium is injected as an impurity into the base gas of hydrogen with the use of a coaxial gun discharge between titanium electrodes. The Ti x ion density at its peak abundance in the plasma is deduced in each discharge from the measured increase in electron density by knowing the temporal charge-state distribution of Ti ions with the use of spectroscopy and assuming charge neutrality.

501,555
PB86-111952 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Atomic and Plasma Radiation Div.
Near-Resonance-Rayleigh Scattering Measurement on a Resonant Laser-Driven Barium Plasma.
Final rept.,
T. J. A. Nee. Jun 85, 5p
Pub. in Jnl. of Applied Physics 57, n11 p4968-4972, 1 Jun 85.

Keywords: *Rayleigh scattering, *Plasma density, Reprints, *Barium plasma, *Ion density.

Near-resonance-Rayleigh scattering is used as a space-time-resolved density probe on a resonant laser-driven barium plasma. Feasibility of this technique was investigated. Comparison to other methods such as absorption technique is made and found to be consistent.

20J. Quantum Theory

501,556
PB85-172195 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Non-Observability of Non-Exponential Decay.
Final rept.,
M. Danos, and A. B. Johnson. 15 Dec 84, 3p
Pub. in Physical Review D 30, n12 p2692-2694, 15 Dec 84.

Keywords: *Radioactivity, Quantum theory, Exponential functions, Reprints, *Unified-field theories, Proton decay, Uncertainty.

The decay of an unstable quantum system is treated using covariant relativistic quantum theory. This way all

ambiguities existing in a nonrelativistic treatment are avoided. As a first example, it is shown that the proton in the present era decays exponentially. Two examples are then considered where the unstable particle is produced in a scattering experiment. It is shown that the observability of non-exponential decay is limited by the time-energy uncertainty relations.

501,557
PB85-183259 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Mechanical Production Metrology Div.
Alternative Interaction Between Spinor and Yang-Mills Fields.
Final rept.,
E. Marx. 1984, 11p
Pub. in Il Nuovo Cimento 81 A, n4 p759-769 1984.

Keywords: *Field theory(Physics), *Quantum theory, Relativity, Reprints, *Yang-Mills theory, Gauge theory, Spinors, Isospin.

A new interaction is introduced between the classical spinor-isospinor field and the Yang-Mills field. This interaction is derived from a Lagrangian density that is invariant under local unimodular transformations. New conserved isovector and isoscalar current densities are found; the isoscalar charge is no longer positive definite, which makes this formalism suitable for use in the context of relativistic quantum mechanics.

501,558
PB85-197705 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Derivation of the Ornstein-Zernike Differential Equation from the BBGKY Hierarchy.
Final rept.,
R. F. Kayser, and H. J. Raveche. 1982, 6p
Pub. in Physical Review A 26, n4 p2123-2128 1982.

Keywords: *Critical point, Correlation, Reprints, *BBGKY equation, *Ornstein-Zernike equation.

The theory of inhomogeneous fluids is applied to a d-dimensional system near its critical point to derive the probability of finding a particle at a distance r from a pair separated by a distance s, given that $r > x_i > s$, where x_i is the correlation length. When this result is used in the BBGKY hierarchy, an approximation-free equation is obtained, from which it follows that the pair correlations for $r > x_i$ satisfy the Ornstein-Zernike differential equation.

501,559
PB85-207116 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymers Div.
Field Theory, Curdling, Limit Cycles and Cellular Automata.
Final rept.,
E. A. Di Marzio. 1984, 11p
Pub. in Jnl. of Statistical Physics 36, n5-6 p897-907 1984.

Keywords: *Field theory(Physics), Relativity, Reprints, Fractals, One dimensional, Nonlinear analysis.

It is suggested that the process of curdling is the pre-eminent question for the science of fractals. A field equation which displays nucleation (curdling) of particles out of a pure radiation field is discussed. The particle formation arises naturally from the non-linear character of the equation rather than from imposed quantization conditions. The relativistically invariant equation is given. It represents material at r,t traveling with the velocity of light in direction (Omega vector). Explicit solutions are given for the case of one dimension. Fields representing particles are obtained and shown to have spacially oscillatory structure with incipient fractal character.

501,560
PB85-222321 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Nuclear Radiation Div.
Chiral Fermions Beyond the Standard Model.
Final rept.,
P. M. Fishbane, S. Meshkov, R. E. Norton, and P. Raymond. 1 Mar 85, 8p
Contracts NSF-PHY81-00257, DE-AS05-81-ER0008
Pub. in Physical Review D 31, n5 p1119-1126, 1 Mar 85.

Keywords: *Fermions, Reprints, Chirality.

A scheme is discussed for constructing anomaly-free, charge-vectorial chiral sets of fermions which acquire masses by coupling to the Higgs doublet of the standard model.

501,561

PB86-102993

Not available NTIS
National Bureau of Standards (NML), Boulder, CO.
Time and Frequency Div.

Around-the-World Relativistic Sagnac Experiment.
Final rept.,

D. W. Allan, M. A. Weiss, and N. Ashby. Apr 85, 2p
Sponsored by Colorado Univ. at Boulder. Dept. of
Physics and Astrophysics.
Pub. in Science 228, p69-70, 5 Apr 85.

Keywords: *Atomic clocks, *Relativity, Reprints,
*Sagnac effect, Global positioning system.

In 1971 Hafele and Keating carried portable atomic clocks east and then west around the world and verified the Sagnac effect, a special relativity effect attributable to the earth's rotation. In the study reported here, observations of the effect were made by using electromagnetic signals instead of portable clocks to make clock comparisons. Global Positioning System satellites transmit signals that can be viewed simultaneously from remote stations on the earth; thus an around-the-world Sagnac experiment can be performed with electromagnetic signals. The effect is larger than that occurring when portable clocks are used. The average error over a 3-month experiment was only 5 nanoseconds.

501,562

PB86-112836

Not available NTIS
National Bureau of Standards (NML), Boulder, CO.
Time and Frequency Div.

Atomic Parity Nonconservation Experiments.
Final rept.,

E. N. Fortson, and L. L. Lewis. 1984, 56p
Pub. in Physics Reports 113, n5 p289-344 1984.

Keywords: *Parity, Bismuth, Lead(Metal), Cesium, Thallium, Hydrogen, Weak interactions, Reprints, Weinberg-Salam gauge model.

A comprehensive review of theoretical and experimental studies of parity nonconservation in atoms is presented. The authors describe measurements in bismuth, lead, cesium, and thallium which collectively provide confirmation of the Weinberg-Salam-Glashow 'standard model' of electroweak unification. Ongoing experiments in hydrogen are discussed as well. The authors examine the unique role of all atomic experiments in distinguishing alternative versions of the standard theory. Finally, the authors include some discussion of experiments which search for permanent atomic electric dipole moments as potential evidence of time-reversal violation in particle interaction.

501,563

PB86-132669

Not available NTIS
National Bureau of Standards (NEL), Boulder, CO.
Electromagnetic Technology Div.

Rochester Gravitational-Wave Detector.
Final rept.,

M. F. Bocko, M. W. Cromar, D. H. Douglass, R. Q. Gram, and W. W. Johnson. 1984, 10p
Pub. in Jnl. of Physics E-Scientific Instruments 17, n8 p694-703 1984.

Keywords: Vibration isolators, Superconductors, Reprints, *Gravitational wave detectors, SQUID devices.

In the paper the authors present the first detailed report of the Rochester cryogenic resonant gravitational wave detector. They describe in detail their transducer which makes use of several features (superconducting, wide band, non-contacting) in a unique combination that already has made it possible to achieve the highest mechanical Q for aluminum in a gravitational wave detector ($Q = 2 \times 10$ to the 7th power). They also present encouraging results of preliminary tests, and show how their detector will be able to achieve a competitive ultimate sensitivity even though the detecting mass is smaller than what is commonly used. They include a detailed analysis of the sensitivity and a description of the procedure for the calibration.

501,564

PB86-136868

Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Thermophysics Div.

Mode Coupling from Linear and Nonlinear Kinetic Equations.

Final rept.,

J. W. Dufty, and R. F. Rodriguez. 1983, 26p
Pub. in Jnl. of Statistical Physics 33, n2 p261-286 Nov 83.

Keywords: *Kinetic theory, Boltzmann equation, Spheres, Reprints, Klimontovich equation, Mode coupling.

The calculation of mode coupling contributions to equilibrium time correlation functions from the nonlinear Boltzmann equation is reconsidered. It is suggested that the use of a nonlinear kinetic equation is not appropriate in the context, but instead such calculations should be reinterpreted in terms of the Klimontovich equation for the microscopic phase space density. For hard spheres the Klimontovich equation is formally similar to the nonlinear Boltzmann equation, and the similarity is exploited to explain the successful calculation of mode coupling effects from the latter. The relationship of the Klimontovich formulation to the linear ring approximation is also established.

501,565

PB86-139813

Not available NTIS
National Bureau of Standards (NML), Boulder, CO.
Quantum Physics Div.

Space Antenna for Gravitational Wave Astronomy.
Final rept.,

J. E. Faller, P. L. Bender, J. L. Hall, D. Hils, and M. A. Vincent. 1985, 7p
Pub. in Proceedings of Colloquium on Kilometric Optical Arrays in Space, Corsica, France, October 23-25, 1984, p157-163 1985.

Keywords: Spacecraft, *Gravitational wave antennas, Gravitational radiation, Gravity waves.

The authors are investigating possible designs for a laser gravitational wave antenna in space using free test masses and heterodyne (interferometric) detection. One possibility is to use baselines about one million km long between three spacecraft in nearly circular one-year orbits about the sun. If the orbit elements are chosen properly, the distances between the spacecraft can be kept constant to roughly 1 part in 1000 without orbit corrections. With milliwatt-transmitted laser power levels and 50 cm diameter optics, a strain sensitivity of 10 to the 19th power/(Hz to the 1/2 power) over at least the period range from 10 to 10,000 seconds appears feasible. The primary goal of the measurements is to observe gravitational radiation associated with present or past interactions of super-massive objects.

501,566

PB86-143906

PC A03/MF A01
National Bureau of Standards (NML), Gaithersburg, MD. Center for Radiation Research.

Irreducible Density Matrices,
M. Danos. Nov 85, 27p NBSIR-85/3270

Keywords: *Quantum theory, Angular momentum, Tensor analysis, *Density matrix, Polarization, SU-2 groups.

An expansion of the density matrix is given into irreducible SU(2) tensors, i.e., into quantities of good angular momentum. These irreducible tensors can be handled by all the powerful tools developed in the context of the handling of angular momentum. As examples, the density matrix of a cryogenically aligned nucleus is derived and the construction of the angular distributions of nuclear reactions in terms of density matrices is demonstrated.

20K. Solid Mechanics

501,567

PB86-128915

Not available NTIS
National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.

Waves, Microstructures, and Effective-Medium Approximation.
Final rept.,

S. K. Datta, and H. M. Ledbetter. 1985, 11p
Sponsored by Defense Advanced Research Projects Agency, Arlington, VA.
Pub. in Mechanics of Dislocations, p213-223 1985.

Keywords: *Microstructure, *Elastic properties, Phase velocity, Plane waves, Wave propagation, Preferred orientation, Anisotropy, Inclusions, Reprints.

Theoretically and experimentally the authors studied phase velocity of a plane wave propagating in an elastic medium with microstructure. Microstructures studied were either inclusions or fibers, which were either aligned or oriented randomly. Preferred orientation of the microstructure causes anisotropic macroscopic physical properties. Here the authors consider the elastic properties. The theoretical model used a wave-scattering approach together with Lax's quasi-crystalline approximation. The model predicts the macroscopic isotropic elastic constants for the case of random orientation and the macroscopic anisotropic elastic constants caused by preferred orientation.

501,568

PB86-129061

Not available NTIS
National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.

Review of Generalized Failure Criteria Based on the Plastic Yield Strip Model.
Final rept.,

R. de Wit. 1981, 27p
Sponsored by Federal Railroad Administration, Washington, DC. Office of Rail Safety Research.
Pub. in Proceedings of National Symposium on Fracture Mechanics (14th), Los Angeles, CA., June 30-July 2, 1981, ASTM STP 791, p1-14 - 1-50.

Keywords: *Pressure vessels, Fracture properties, Mechanical properties, Cracks, Failure, Collapse, Fracture(Mechanics).

A review is given of the failure criteria developed by Hahn and Sarrafe for through-cracked pressure vessels, whereby they established three failure categories. This work was based on the Dugdale and Bilby-Cottrell-Swinden (D-BCS) model for the crack-tip opening displacement (CTOD) in an infinite plate. The model was extended in an approximate way by Heald-Spink-Worthington (D-BCS-HSW) to finite geometries and structures by combining the effects of plasticity and geometry as multiplicative factors. In this paper the criteria of Hahn and Sarrafe are extended to the D-BCS-HSW model. The three failure categories are relabelled: (1) linear-elastic fracture mechanics (LEFM), (2) elastic-plastic fracture mechanics (EPFM), and (3) plastic collapse (PC).

501,569

PB86-138104

Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Mathematical Analysis Div.

Fatigue Research: Needs and Opportunities.
Final rept.,

J. T. Fong. 1985, 5p
Pub. in ASTM (American Society for Testing and Materials) Standardization News 13, n11 p59-63 1985.

Keywords: *Fatigue(Materials), Mechanical properties, Crack propagation, Fatigue tests, Cracking(Fracturing), Reprints.

The significance of fatigue research in engineering and materials science is stated in simple terms through a look at the goals of research and its benefits to society. An overview of the research progress during the last 30 years is given in a historical perspective dating back to as far as the 1840's. The driving forces for research support from the industry and the user community are introduced to place the concept of 'research needs' in a practical setting. Technical difficulties in moving fatigue toward a more scientific basis are discussed.

501,570

PB86-143856

PC A04/MF A01
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Mfg. Engineering.

Dynamic Green's Functions of an Infinite Plate - A Computer Program,
N. N. Hsu. Nov 85, 67p NBSIR-85/3234

Keywords: *Plates(Structural members), *Greens function, *Computer programs, Nondestructive tests, Elastic waves, Waveforms, Fortran, Convolution integrals, *Acoustic emissions.

The report is a FORTRAN program to compute the Green's functions of an infinite plate. The Green's function, $G(ij)(x_i, x_j, t)$, is defined as the i th component of the displacement at x due to a point force of step-

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function time dependency acting at x_i in the j th direction initiated at $t=0$. The Green's function is the fundamental solution of the transient elastic wave propagation problem. In general, the displacement field $u(x_i, x_j, t)$ at x due to a point force of arbitrary time dependence acting at x_i can be computed by a convolution integration. Displacement produced by a dynamic force distributed over a finite area can also be computed by numerical integration using the Green's function as the kernel of the integral over the finite area. The computer program is made available mainly for its application to calibrate acoustic emission systems and sensors.

20L. Solid-State Physics

501,571
PB85-184836 PC A08/MF A01
National Bureau of Standards, Gaithersburg, MD. Reactor Radiation Div.
NBS (National Bureau of Standards) Reactor: Summary of Activities July 1983 through June 1984.
Technical note,
F. J. Shorten. Feb 85, 163p NBS/TN-1207
Also available from Supt. of Docs as SN003-003-02643-3. See also PB83-218636.

Keywords: *Neutron beams, *Research reactors, Nuclear research and test reactors, Neutron irradiation, Neutron activation analysis, Neutron diffraction, Neutron radiography, Materials tests, Crystal structure.

This report summarizes all those programs which depend on the NBS reactor. It covers the period from July 1983 through June 1984. 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, radiation effects studies, neutron radiography, and nondestructive evaluation.

501,572
PB85-186997 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Semiconductor Devices and Circuits Div.
Comparison of Theoretical and Empirical Lifetimes for Minority Carriers in Heavily Doped Silicon.
Final rept.,
H. S. Bennett. 1984, 5p
Pub. in Solid-State Electronics 27, n10 p893-897 1984.

Keywords: *Silicon, Field effect transistors, Semiconductor doping, Reprints, *Minority carriers, *Carrier lifetime, *Semiconductors, Bipolar transistors.

The minority carriers determine essential electrical characteristics of bipolar devices and bipolar-like parasitic paths in field effect devices. The electrical behavior of such devices is frequently described by detailed device models. Compared to the other input parameters for detailed device models, the minority carrier lifetimes due to traps or defects as functions of doping density have great uncertainty. A major finding in this paper is that the commonly used empirical expressions for the lifetime due to defects may not give correct results when included in detailed models of shallow, heavily doped silicon emitters.

501,573
PB85-187375 Not available NTIS
National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.
Changes in Stress Intensity with Dislocation Emission from a Crack.
Final rept.,
I. H. Lin, and J. P. Hirth. 1984, 4p
Pub. in Philosophical Magazine A, 50, n6 pL43-L46 1984.

Keywords: *Stresses, Intensity, Dislocations(Materials), Crack propagation, Reprints.

Dislocation emission from a sharp crack changes it to a mixed defect with both crack and superdislocation character. The dislocation component can either enhance or retard the tendency for crack propagation.

501,574
PB85-189397 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Semiconductor Materials and Processes Div.

High-Frequency Transient-Resistance Spectroscopy of Deep Levels in Si GaAs.

Final rept.,
A. C. Seabaugh, M. I. Bell, R. D. Larrabee, and J. D. Oliver. 1984, 9p
Pub. in Proceedings of Semi-Insulating 3-Materials Kah-nee-ta 1984, p437-445 1984.

Keywords: *Gallium arsenides, Chromium, Reprints, *Deep level transient spectroscopy, *Photoresistance deep level transient spectroscopy, Doped materials.

A new photoinduced transient-resistance technique is used to characterize deep levels in semi-insulating GaAs. In this technique, termed photoresistance deep-level transient spectroscopy (PR-DLTS), an optical pulse is used to generate excess carriers which are trapped by deep levels in the material. The ac resistance of the specimen is monitored, and the resistance transient which occurs after the illumination ends is signal processed in the same way as the capacitance transient in conventional DLTS. Comparison of this technique with the dc current-transient measurement, photoinduced transient spectroscopy (PITS), shows that it is sensitive to the same trapping/detrapping phenomena. PR-DLTS data for the Cr-related deep level is consistent with published DLTS results. Results are reported for materials grown by the horizontal Bridgman method and by the liquid-encapsulated Czochralski technique, both with and without chromium doping. Nineteen specimens from ten different manufacturers are compared.

501,575
PB85-189470 Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div.
Investigation of a Practical Superconductor with a Copper Matrix.
Final rept.,
F. R. Fickett. Sep 84, 60p
Sponsored by International Copper Research Association, Inc., New York. See also PB-299762.
Pub. in Proceedings of International Copper Research Association Annual Report, 57p 1984.

Keywords: *Superconductors, Copper, Composite materials, Niobium intermetallics, Tin intermetallics, Wire, Reprints, Copper matrix composites.

The report summarized the work performed on four INCRA projects covering a span of about six years. The main goal of the work was to investigate the in-situ superconductors, those produced by the relatively rapid cooling of a melt containing essentially non-miscible components. The component with the higher melting point precipitates out as small particles during the cooling. Subsequent drawing of the resulting boule results in fine filaments of this material (the superconductor) in the lower-melting matrix (usually oxygen-free copper or a copper-tin alloy).

501,576
PB85-196111 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Interaction Effects in Disordered Landau-Level Systems in Two Dimensions.
Final rept.,
S. M. Girvin, M. Jonson, and P. A. Lee. 1982, 9p
Pub. in Physical Review B: Condensed Matter 26, n4 p1651-1659, 1 Aug 82.

Keywords: *Electron gas, *Coulomb interactions, Magnetic fields, Reprints, Density of states, Two dimensional.

Interaction effects in the disordered two dimensional electron gas are considered in the regime of high magnetic field and low temperature. Logarithmic temperature corrections to the density of states and the conductivity are obtained. When Hartree corrections are included, good agreement with the experimental results of Paalanen, et al. is obtained.

501,577
PB85-196228 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Reversible Step Rearrangement and Segregation on Nickel Surface at the Curie Temperature.
Final rept.,
T. Jach, and J. C. Hamilton. 1982, 8p
Pub. in Physical Review B: Condensed Matter 26, n7 p3766-3773, 1 Oct 82.

Keywords: *Ferromagnetic materials, *Nickel, *Surfaces, Phase transformations, Single crystals, Curie temperature, Carbon, Separation, Reprints.

Reversible step period rearrangement and carbon segregation have been observed on clean nickel single-crystal surfaces whose bulk is also relatively free of impurities. The temperature of these transitions which are 35K wide, appears to be the nickel Curie temperature, as determined by simultaneous LEED, Auger, and permeability measurements on nickel stepped and flat (111) surfaces. The observation of segregated carbon in carbide form (isolated carbon atoms) indicates an unusual bonding state of C to the surface below the Curie temperature. Measured carbon coverages indicate a change greater than 0.2eV per carbon atom in the heat of segregation at the Curie point.

501,578
PB85-196236 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Integral Equation Approach to the Inclusion Problem of Elasto-Plasticity.
Final rept.,
W. C. Johnson, and J. K. Lee. 1982, 7p
Pub. in Jnl. of Applied Mechanics 49, n2 p312-318 Jun 82.

Keywords: *Elastic properties, *Plastic properties, *Integral equations, Deformation, Strains, Stresses, Reprints, Pearson density functions.

An integral equation approach is derived for the calculation of the elasto-plastic strain field associated with a transformed inclusion of constant stress-free transformation strain and for an inhomogeneity when the far stress field remains elastic. The assumptions of a coherent precipitate and the deformation theory of plasticity are employed although any yield condition and flow rule can be chosen. The complexity of the integral equation is such as to necessitate an iterative solution scheme. The technique is applied to a spherical precipitate in a uniform elastic stress field where associated stress and strain fields and plastic zone are calculated. The nature of the plastic relaxation process compares qualitatively with two dimensional plane stress behavior. Extension of this technique to the nonaxisymmetric problem is also examined.

501,579
PB85-196277 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Radial Distribution Studies in A Diamond Anvil Pressure Cell (Amorphous Fe-W).
Final rept.,
R. G. Munro, S. Block, F. A. Mauer, and G. J. Piermarini. 1982, 2p
Pub. in Jnl. of Applied Physics 53, n10 p7080-7081 Oct 82.

Keywords: X ray diffraction, Load cells, Iron alloys, Tungsten alloys, Reprints, *Radial distribution functions, Amorphous materials, High pressure.

High pressure radial distribution studies using energy dispersive x-ray diffraction have been performed for the first time in a diamond anvil pressure cell (DAPC). The differential radial distribution function (RDF) and the associated reduced structure factor (SF) have been determined for the amorphous metal Fe-W (56 wt.% W) at room temperature and at pressures of 0, 0.3, 3.6, 7.3, and 10.5 GPa.

501,580
PB85-197572 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Observation of Spin Waves in Pd(1.5% Fe).
Final rept.,
J. W. Lynn, J. J. Rhyne, and J. I. Budnick. 1982, 3p
Sponsored by American Inst. of Physics, New York and Institute of Electrical and Electronics Engineers, Inc., New York.
Pub. in Proceedings of Annual Conference on Magnetism and Magnetic Materials (27th), Atlanta, Ga., November 10-13, 1981, Jnl. of Applied Physics 53, n3 pt2 Mar 84.

Keywords: *Ferromagnetic materials, *Palladium alloys, *Iron containing alloys, *Magnons, Neutron scattering, Magnetic moments, Cryogenics, *Spin waves.

Inelastic neutron scattering measurements have been carried out on the 'giant-moment' alloy system Pd(1.5% Fe), which is in the dilute ferromagnetic regime. Below the Curie temperature of 67K relatively well defined spin wave excitations have been observed in the small wavevector region ($Q < 0.14/\text{\AA}$).

The dispersion of these excitations is consistent with the quadratic relation $E = D(Q \supset 2)$ expected for an isotropic ferromagnet, with $D = 40 \text{ meV-(Å} \supset 2)$ at a temperature of the 40K. With increasing temperature, the spin waves are found to renormalize in energy, and broaden rapidly both with increasing Q and increasing temperature.

501,581
PB85-197580 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Effects of Inhomogeneous Strain in Ferroelectric Crystals Near Their Phase Transitions.
Final rept.,
G. M. Loicono, M. Delfino, A. Shaulov, W. A. Smith, and M. I. Bell. 1980, 4p
Pub. in *Ferroelectrics* 29, n3-4 p181-184 1980.

Keywords: *Ferroelectric crystals, *Specific heat, *Strains, Phase transformations, Pyroelectricity, Reprints, *Ammonium lithium sulfates, *Gadolinium molybdates, *Terbium molybdates, *Nickel borate bromides, Temperature dependence.

Measurements of the temperature dependence of the heat capacity in LiNH_4SO_4 , $\text{Gd}_2(\text{MoO}_4)_3$, $\text{Tb}_2(\text{MoO}_4)_3$ and $\text{Ni}_3\text{B}_7\text{O}_{13}\text{Br}$, near their ferroelectric phase transitions, exhibit multiple peaking. An explanation of this behavior, based on strains induced during crystal growth and/or sample fabrication, is described.

501,582
PB85-206712 (Order as PB85-206324, PC A13/MF A01)
University of Southern California, Los Angeles. Center for Laser Studies.
Optical Absorption in the Band Gap in High Purity Silicon,
R. T. Swimm. Apr 85, 2p
Included in OM85: Basic Properties of Optical Materials. Summaries of Papers, p158-159 Apr 85.

Keywords: *Silicon, *Energy bands, Band structure of solids, Energy gap, Single crystals, Near infrared radiation, Laser radiation, Absorption coefficients, Calorimetry.

Calorimetric measurement of weak optical absorption of laser illumination by solid samples is a well established method. The possibility of applying such methods to the study of deep level impurities has been discussed in the literature (1,2), but little data has been published. In this paper, some of the many difficulties and constraints in applying calorimetry to the study of deep level impurities are discussed. The goal of the present study was to determine the energy of a deep level with respect to either the valence or conduction band edge. In order to do this it is necessary to measure the photolionization or photoneutralization cross section as a function of photon energy.

501,583
PB85-206803 (Order as PB85-206324, PC A13/MF A01)
Max-Planck-Inst. fuer Festkoerperforschung, Stuttgart (Germany, F.R.).
Dielectric Function and Interband Transitions in Semiconductors,
M. Cardona. Apr 85, 6p
Included in OM85: Basic Properties of Optical Materials. Summaries of Papers, p188-193 Apr 85.

Keywords: *Semiconductors(Materials), *Energy bands, Optical properties, Silicon, Germanium, Tin, Ellipsometry, Cadmium manganese tellurides, Cadmium mercury tellurides, Germanium sulfides.

No abstract available.

501,584
PB85-206811 (Order as PB85-206324, PC A13/MF A01)
National Bureau of Standards (NEL), Gaithersburg, MD. Semiconductor Materials and Processes Div.
Band Structure and Density of States Changes for Doped Gallium Arsenide,
H. S. Bennett. Apr 85, 4p
Included in OM85: Basic Properties of Optical Materials. Summaries of Papers, p194-197 Apr 85.

Keywords: *Gallium arsenide, *Energy bands, Band structure of solids, Absorption, Density of states, Doped materials.

The paper contains calculations of the changes in the band structure and density of states for both n-type

and p-type doped GaAs. These band structure changes may be applied to optical properties such as absorption, luminescence, and refractive index. The application to absorption is given here.

501,585
PB85-206852 (Order as PB85-206324, PC A13/MF A01)
Ohio State Univ., Columbus.
Picosecond Carrier Dynamics in alpha-Si,
A. I. D'Souza, M. G. Roe, and P. E. Wigen. Apr 85, 4p
Prepared in cooperation with Pennsylvania State Univ., University Park. Materials Research Lab.
Included in OM85: Basic Properties of Optical Materials. Summaries of Papers, p218-221 Apr 85.

Keywords: *Silicon, *Charge carriers, Carrier mobility, Energy bands, Dynamics, Picosecond pulses, Density of states.

The observations suggest that the large density of states in the gap in $\alpha\text{-Si}$ provides a fast and easy non-radiative channel for the decay of charge carriers out of the conduction band. This conclusion is derived from the exponential decay in the reflectance which is interpreted as indicating the dominance of monomolecular non-radiative recombination, with bimolecular radiative recombination relatively unimportant in sputtered $\alpha\text{-Si}$ at $T = 300 \text{ K}$ up to 900 ps.

501,586
PB85-206902 (Order as PB85-206324, PC A13/MF A01)
Hughes Research Labs., Malibu, CA.
Measurement of Dielectric Properties of $\text{KTa}(1-x)\text{Nb}(x)\text{O}_3$ at Millimeter Wavelengths,
D. Rytz, M. B. Klein, B. Bobbs, M. Matloubian, and H. Fetterman. Apr 85, 4p
Prepared in cooperation with California Univ., Los Angeles. Dept. of Electrical Engineering.
Included in OM85: Basic Properties of Optical Materials. Summaries of Papers, p234-237 Apr 85.

Keywords: *Ferroelectric crystals, *Dielectric properties, Millimeter waves, Measurement, *Potassium tantalate niobates.

Mixed crystals of $\text{KTa}(1-x)\text{Nb}(x)\text{O}_3$ or KTN are well known ferroelectrics whose transition temperatures $T(c)$ can be adjusted between -273 and 430 degrees C by varying the Nb concentration x . In the present work, the authors report on dielectric measurements in the 60-95 GHz range for crystals with $x = 0.20, 0.09, 0.025, 0$ and $T(c) = -103, -183, -238$ degrees C respectively (for $x = 0$, i.e. pure $\text{KTaO}_3(c)$, there is no transition).

501,587
PB85-207389 Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div.
Survey of Chaos in the Rf-Biased Josephson Junction.
Final rept.,
R. L. Kautz, and R. Monaco. 1 Feb 85, 15p
Pub. in *Jnl. of Applied Physics* 57, n3 p875-889, 1 Feb 85.

Keywords: *Josephson junctions, Superconductivity, Reprints, *Chaos, Voltage standards.

Chaotic behavior in the rf-biased Josephson junction is studied through digital simulations of the Stewart-McCumber model. Chaotic states are characterized by Poincare sections, Liapunov exponents, and power spectra. Models are presented which explain some features of the chaotic spectra. The parameter range over which chaotic behavior occurs is determined empirically for a broad range of dc bias, rf bias, and the hysteresis parameter for a fixed rf frequency. It is shown that chaos does not occur if either the dc bias or the rf bias is very large. An attempt is made to explain the boundaries of the chaotic region in terms of simple models for chaotic behavior.

501,588
PB85-219855 Not available NTIS
Purdue Univ., Lafayette, IN.
Electrical Resistivity of Selected Elements,
P. D. Desai, T. K. Chu, H. M. James, and C. Y. Ho. c1984, 28p
Sponsored by National Bureau of Standards, Gaithersburg, MD.
Included in *Jnl. of Physical and Chemical Reference Data*, v13 n4 p1069-1096 1984. Available from Ameri-

can Chemical Society, 1155 Sixteenth St., N.W., Washington, DC 20036.

Keywords: *Electrical resistivity, *Hafnium, *Molybdenum, *Tantalum, *Tungsten, *Zinc, Graphs(Charts), Melting point, Metals, Experimental design, Cryogenics, Temperature dependence.

The work compiles, reviews, and discusses the available data and information on the electrical resistivity of hafnium, molybdenum, tantalum, tungsten, and zinc, and presents the recommended values resulting from critical evaluation, correlation, analysis, and synthesis of the available data and information. The recommended values presented are both uncorrected and also corrected for the thermal expansion of the material and cover the temperature range from 1 K to above the melting point into the molten state. The estimated uncertainties in most of the recommended values are about + or - 2% to + or - 10%.

501,589
PB85-219863 Not available NTIS
Purdue Univ., Lafayette, IN.
Electrical Resistivity of Vanadium and Zirconium,
P. D. Desai, H. M. James, and C. Y. Ho. c1984, 34p
Sponsored by National Bureau of Standards, Gaithersburg, MD.
Included in *Jnl. of Physical and Chemical Reference Data*, v13 n4 p1097-1130 1984. Available from American Chemical Society, 1155 Sixteenth St., N.W., Washington, DC 20036.

Keywords: *Electrical resistivity, *Vanadium, *Zirconium, Graphs(Charts), Tables(Data), Experimental design, Melting point, Metals, Thermal expansion, Purity, Cryogenics, Temperature dependence.

The work compiles, reviews, and discusses the available data and information on the electrical resistivity of vanadium and zirconium and presents the recommended values resulting from critical evaluation, correlation, analysis, and synthesis of the available data and information. The recommended values presented are uncorrected and also corrected for the thermal expansion of the material and cover the temperature range from 1 K to above the melting point into the molten state. The estimated uncertainties in most of the recommended values are about + or - 2% to + or - 5%.

501,590
PB85-219871 Not available NTIS
Purdue Univ., Lafayette, IN.
Electrical Resistivity of Aluminum and Manganese,
P. D. Desai, H. M. James, and C. Y. Ho. c1984, 42p
Sponsored by National Bureau of Standards, Gaithersburg, MD.
Included in *Jnl. of Physical and Chemical Reference Data*, v13 n4 p1131-1172 1984. Available from American Chemical Society, 1155 Sixteenth St., N.W., Washington, DC 20036.

Keywords: *Electrical resistivity, *Aluminum, *Manganese, Thermal expansion, Melting point, Metals, Graphs(Charts), Tables(Data), Purity, Cryogenics, Temperature dependence.

The work compiles, reviews, and discusses the available data and information on the electrical resistivity of aluminum and manganese and presents the recommended values resulting from critical evaluation, correlation, analysis, and synthesis of the available and information. The recommended values presented are uncorrected and also corrected for the thermal expansion of the material and cover the temperature range from 1 K to above the melting point into the molten state for aluminum and to 700 K for manganese. The estimated uncertainties in most of the recommended values are about + or - 2% to + or - 5%.

501,591
PB85-227643 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Radiation Physics Div.
Connection between Surface Magnetism and Electronic Structure of Oxygen on Ni(110) (Invited).
Final rept.,
A. Seiler, C. S. Feigerle, J. L. Pena, R. J. Celotta, and D. T. Pierce. 15 Apr 85, 3p
Sponsored by National Science Foundation, Washington, DC., and Office of Naval Research, Arlington, VA.
Pub. in *Jnl. of Applied Physics* 57, n1 p3638-3640, 15 Apr 85.

Field 20—PHYSICS

Group 20L—Solid-State Physics

Keywords: *Nickel, *Magnetism, *Surfaces, Chemisorption, Oxidation, Reprints, *Electronic structure, Photoelectron spectroscopy.

The d-band holes which give rise to ferromagnetism in Ni can be directly observed by spinpolarized inverse photoelectron spectroscopy (SPIES). Only incident electrons polarized in the minority spin direction can fall into unfilled minority spin states and radiate a detected photon. On dissociative chemisorption of O₂ one observes a reduction in the number of minority spin d holes. It is this change in electronic structure which gives rise to a decrease in magnetization. A background of minority and majority spin states remains essentially unchanged. Further exposure to oxygen causes formation of NiO; the surface magnetization goes to zero, and a completely different SPIES spectrum is observed. The relative importance of d electrons and s, p electrons in chemisorptive bonding on Ni has been much discussed. These data suggest that the d states interact strongly with the oxygen and that this interaction has a profound influence on the surface magnetism.

501,592
PB85-230746 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Semiconductor Devices and Circuits Div.
Heavy Doping Effects on Bandgaps, Effective Intrinsic Carrier Concentrations and Carrier Mobilities and Lifetimes.
Final rept.,
H. S. Bennett. 1985, 9p
Pub. in Solid-State Electronics 28, n1/2 p193-200 1985.

Keywords: *Semiconductor doping, Mathematical models, Computerized simulation, Donor materials, Energy gap, Carrier mobility, Transistors, Reprints, Carrier lifetime.

Conventional device physics in most computer models of transistors may not predict correctly the measured electrical performance for shallow, heavily doped transistors. This paper presents improved concepts for numerical simulations of solid-state devices with donor densities up to 3×10^{19} to the 20th power/cc and junction depths as small as 1 micrometer. These improved concepts pertain to bandgap narrowing, effective intrinsic carrier concentrations, and carrier mobilities and lifetimes.

501,593
PB85-230852 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Conductivity Mechanisms in the Superionic Phases of AgI and Ag₂S as Determined by Neutron Diffraction.
Final rept.,
R. J. Cava, F. Reidinger, and B. J. Wuensch. 1979, 5p
Pub. in Proceedings of the International Conference on Fast Ion Transport in Solids - Electrolytes and Electrodes, Lake Geneva, Wisconsin, May 19-27, 1979, p217-220.

Keywords: *Silver iodide, *Silver sulfides, Neutron diffraction, *Superionic conductivity, *Ionic conductivity.

Both alpha AgI and beta Ag₂S have a BCC anion array. Neutron diffraction experiments indicate that silver ion transport in alpha AgI is characterized by continuous independent ion motion between nearest neighbor tetrahedral sites, whereas that in beta Ag₂S is dominated by silver-silver interaction. The differences are attributed to mobile ion concentration and cation-anion bonding characteristics.

501,594
PB86-111879 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Effect of Bandgap Narrowing on Diffusion Processes in Silicon.
Final rept.,
J. R. Lowney. 1982, 7p
Sponsored by Electrochemical Society, Inc., Pennington, N.J. Electronics Div.
Pub. in Proceedings of the Very Large Scale Integration Science and Technology International Symposium (1st), Detroit, MI., October 18-21, 1982, v82-87, p123-129.

Keywords: *Silicon, *Energy gap, Integrated circuits, Energy bands, *Very large scale integration, Density of states.

As the dimensions of devices become smaller, the effect of bandgap narrowing, which occurs in silicon as a result of heavy doping, becomes increasingly more important. The diffusion coefficients of dopant ions depend strongly on the ratio of the majority carrier density to the intrinsic carrier density, which increases with decreasing energy gap. The authors have previously developed a model, restricted to donors, which accounts for the bandgap narrowing observed optically at 35 and 300 K. These results have been extended to the case of a donor density of 1.0×10^{19} to the 20th power/cc at 1100C, for which our model predicts a bandgap reduction of 123 meV. However, the intrinsic carrier density is increased by only 15 percent because the perturbed bands are nonparabolic. The authors conclude that bandgap narrowing resulting from heavy doping has a much smaller effect on diffusion coefficients than predicted by prior models based on impurity bands.

501,595
PB86-112117 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Reactor Radiation Div.
Low-Temperature Spin Correlations and Spin Dynamics in Diluted Magnetic Semiconductors.
Final rept.,
T. M. Giebultowicz, J. J. Rhyne, W. Y. Ching, and D. L. Huber. Apr 85, 3p
Sponsored by National Science Foundation, Washington, DC.
Pub. in Jnl. of Applied Physics 57, n1 p3415-3417, 15 Apr 85.

Keywords: Neutron scattering, Magnons, Reprints, *Magnetic semiconductors, *Cadmium manganese tellurides, *Semiconductors, Heisenberg antiferromagnets.

Neutron scattering measurements of static and dynamic spin correlations in the semimagnetic semiconductor Cd(0.35)Mn(0.65)Te are reported and compared to computer simulations for a dilute Heisenberg fcc antiferromagnet that is the model analog of Cd(1-x)Mn(x)Te.

501,596
PB86-112125 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.
Collective-Excitation Gap in the Fractional Quantum Hall Effect.
Final rept.,
S. M. Girvin, A. H. MacDonald, and P. M. Platzman. Feb 85, 3p
Pub. in Physical Review Letters 54, n6 p581-583, 11 Feb 85.

Keywords: *Hall effect, Excitation, Reprints, *Fractional quantum Hall effect, *Quantum Hall effect.

The authors present a theory of the collective excitation spectrum in the fractional quantum Hall-effect regimes, in analogy with Feynman's theory for helium. The spectrum is in excellent quantitative agreement with the numerical results of Haldane. Within this approximation the authors prove that a finite gap is generic to any liquid state in the extreme quantum limit and that in this single-mode approximation gapless excitations can arise only as Goldstone modes for ground states with broken translation symmetry.

501,597
PB86-112778 Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div.
Further Investigations of the Solid-Liquid Reaction and High-Field Critical Current Density in Liquid-Infiltrated Nb-Sn Superconductors.
Final rept.,
M. Hong, D. M. Maher, M. B. Ellington, F. Hellman, and T. H. Geballe. 1985, 4p
Sponsored by David W. Taylor Naval Ship Research and Development Center, Bethesda, MD., and Department of Energy, Washington, DC. Office of Fusion Energy.
Pub. in IEEE (Institute of Electrical and Electronics Engineers) Transactions of Magnetism MAG-21, n2 p771-774 Mar 85.

Keywords: *Superconductors, Niobium intermetallics, Tin intermetallics, Reprints, *Niobium tin, Critical current.

Superior superconducting properties, such as high J(c)'s and T(c)'s, have been obtained from reacted

liquid-infiltrated Nb-Sn composite wires. These excellent properties are attributed to the chemistry and structure of the material, which is prepared by a unique solid (Nb) - liquid (Sn) reaction. From heat capacity measurements, sharp bulk superconducting transitions of the A15 phase occur at 17.2-18 K and the weight fraction of A15 in the composite wire is about 23%. Analytical electron microscopy techniques have shown that the microstructure of these conductors consists of alternating large-grain and small-grain filaments.

501,598
PB86-115540 Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div.
Effect of Uniaxial Strain on the Critical Current and Critical Field of Chevrel Phase PbMo₆S₈ Superconductors.
Final rept.,
J. W. Ekin, T. Yamashita, and K. Hamasaki. 1985, 4p
Sponsored by Department of Energy, Washington, DC. Office of Fusion Energy.
Pub. in IEEE (Institute of Electrical and Electronics Engineers) Transactions on Magnetism MAG-21, n2 p474-477 Mar 85.

Keywords: *Superconductors, *Critical field, Strains, Reprints, *Critical current, *Lead molybdenum sulfides.

The first measurements of the effect of uniaxial strain on the critical current of a Chevrel phase superconductor, PbMo₆S₈, have been obtained at 4.2 K in magnetic fields from 2 T to 24 T. The data show there is a very significant reversible effect of elastic strain on the critical current of PbMo₆S₈, comparable in magnitude to that observed in Nb₃Sn. This is because both the peak pinning force and upper critical field are very sensitive to elastic strain. A correlation is noted between the elastic strain effect, radiation sensitivity, and crystal phase.

501,599
PB86-119419 Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Fields Div.
Differences between Spin Glasses and Ferroglasses: Pd-Fe-Si.
Final rept.,
R. B. Goldfarb, K. V. Rao, and H. S. Chen. 1985, 3p
Pub. in Solid State Communications 54, n9 p799-801 1985.

Keywords: Phase transformations, Ferromagnetism, Paramagnetism, Palladium, Iron, Silicon, Reprints, *Spin glass state, Magnetic susceptibility.

Near the multicritical point in the magnetic phase diagram, some alloys that appear to be simple spin glasses actually have an intermediate ferro-magnetic-like state between the high-temperature paramagnetic and low-temperature spin-glass states. The temperature dependences of the imaginary component of a.c. susceptibility and d.c. magnetization are presented to illustrate the subtle experimental differences between spin glasses and these ferroglasses.

501,600
PB86-119435 Not available NTIS
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Technology Div.
Magnetic Hysteresis and Complex Susceptibility as Measures of AC Losses in a Multifilamentary NbTi Superconductor.
Final rept.,
R. B. Goldfarb, and A. F. Clark. 1985, 4p
Sponsored by Air Force Office of Scientific Research, Bolling AFB, DC.
Pub. in IEEE (Institute of Electrical and Electronics Engineers) Transactions on Magnetism MAG-21, n2 p332-335 Mar 85.

Keywords: *Superconductors, *Magnetic hysteresis, Alternating current, Magnetic permeability, Niobium, Titanium, Losses, Reprints, *Magnetic susceptibility, Critical current.

Magnetization and ac susceptibility of a standard NbTi superconductor were measured as a function of longitudinal dc magnetic field. The ac-field-amplitude and frequency dependences of the complex susceptibility are examined. The magnetization is related to the susceptibility by means of a theoretical derivation based on the field dependence of the critical current density.

Hysteresis losses, obtained directly from dc hysteresis loops and derived theoretically from ac susceptibility and critical current density, were in reasonable agreement.

501,601
PB86-122942 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Operations Research Div.
Generalized Theory of Neutron Scattering from Hydrogen in Metals.
Final rept.,
R. C. Casella. 1983, 10p
Pub. in *Physical Review B: Condensed Matter* 28, n6 p2927-2936, 15 Sep 83.

Keywords: *Neutron scattering, *Hydrogen, Metals, Energy bands, Reprints.

A recent analysis by the author of inelastic scattering of neutrons from dilute hydrogen in terms of coherent itinerant-proton energy bands is generalized to include incoherent processes such as the spontaneous decay of the proton from excited-oscillator states to the ground state, as well as incoherent hopping among excited local-oscillator states centered at neighboring interstitial occupancy sites. Similarly, the analysis of Chudley and Elliott of quasielastic neutron scattering and its extension by Rowe, Skold, Flowtow, and Rush are generalized to include coherent hopping (band transport) in the self-correlation function describing motion of the proton among neighboring oscillator ground states (and, when applicable, among excited states). The general formalism developed here encompasses quasielastic and inelastic scattering and allows for the coexistence of coherent and incoherent processes. At each level of complexity, the expressions obtained for the cross sections are shown to reduce to earlier results in the limits when either the coherent or the incoherent contributions to the neutron bandwidths can be ignored.

501,602
PB86-124096 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Polymer Science and Standards Div.
Numerical Analysis of the Thermal Pulse Experiment (Dielectric Polarization Distributions Measurement).
Final rept.,
F. I. Mopsik, and A. S. DeReggi. 1980, 9p
Pub. in *Proceedings of 1980 Annual Report Conference on Electrical Insulation and Dielectric Phenomena*, Boston, MA., October 26-29, 1980, p251-259.

Keywords: *Polarization(Charge separation), Thermal radiation, Electrets, Fourier analysis, Computer applications, Transients.

The thermal pulse experiment has been presented as a way of investigating polarization distributions in poled materials. The method involves measuring the electrical response to a thermal pulse applied to one surface of a sample by a light flash. The Fourier analysis that the authors developed for the thermal pulse experiment has been used for the development of a computer program to analyze experimental data. The development of this program has led to a better understanding of the actual experiment, both as to experimental requirements and the results that are obtainable for the desired polarization distribution. The authors present the requirements on the sample cell, the effect of finite light pulses, and the optimum time sampling. They also show what the best possible result can be for the spatial distribution of polarization and how close one can come to it. Both actual and calculated data will be presented to illustrate their results.

501,603
PB86-124781 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD.
Understanding Materials Reliability - The Mechanisms of Fracture.
Final rept.,
R. M. Thomson. 1980, 8p
Pub. in *DARPA/AFML (Defense Advanced Research Projects Agency/Air Force Materials Lab.) Review of Progress in Quantitative Nondestructive Evaluation*, La Jolla, CA., July 8-13, 1979, p159-166 1980.

Keywords: *Fractures(Materials), Fracture properties, Brittleness, Fatigue(Materials), Ductility, Plastic properties, *Fracture(Mechanics), Nondestructive evaluation.

For the benefit of the NDE community, a personal view will be given of the current status of our understanding of materials fracture. The discussion will include a general description of the physical and chemical processes which occur when a solid under load possesses a crack. A physical picture is presented of the role of plasticity. The basic question of ductile vs brittle response of the solid is addressed and recent ideas and progress is reviewed. Time dependence, and its manifestation in materials fatigue are briefly described. The implications for NDE are on two levels: (1) new insight generated by fundamental advances in the science of materials reliability will lead to new NDE tools; and (2) NDE techniques can and should be applied to further the fundamental understanding of reliability.

501,604
PB86-128154 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Semiconductor Materials and Processes Div.
Band-Gap Narrowing in the Space-Charge Region of Heavily Doped Silicon Diodes.
Final rept.,
J. R. Lowney. 1985, 5p
Pub. in *Solid-State Electronics* 28, n1/2 p187-191 1985.

Keywords: *Energy gap, *Silicon, Semiconductor diodes, Space charge, Semiconductor doping, Reprints, Density of states.

The densities of states of the valence and conduction bands have been calculated in the space-charge region of a heavily doped linearly graded p-n junction silicon diode. Both the donor and acceptor densities were chosen to be equal to 6.2×10^{18} to the 18th power/cc. The results showed the emergence of band tails which penetrated deeply into the energy gap and accounted for the band-gap narrowing observed in such a diode by analysis of capacitance vs voltage measurements of the built-in voltage.

501,605
PB86-128733 PC A08/MF A01
National Bureau of Standards (NEL), Boulder, CO. Electromagnetic Fields Div.
Development of Standards for Superconductors, Interim Report January 1982-December 1983,
L. F. Goodrich, J. V. Minervini, A. F. Clark, F. R. Fickett, and J. W. Ekin. Jan 85, 168p NBSIR-85/3027
Contract DE-AI01-76PR06010
See also PB83-110296. Sponsored by Department of Energy, Washington, DC.

Keywords: *Superconductors, *Standards, Measurement, Losses, Critical current, Superconducting wires.

A cooperative program with the Department of Energy, the National Bureau of Standards, and private industry is in progress to develop standard measurement practices for use in large scale applications of superconductivity. The goal is the adoption of voluntary standards for the critical parameters and other characterizations of practical superconductors. Progress for the period January 1982 through December 1983 is reported. The major effort was the procurement, selection, and certification of the first superconducting wire for critical current measurements as a Standard Reference Material (SRM 1457). Other work reported here includes: effect of geometry on current transfer; lap-joint resistance; and ac losses.

501,606
PB86-132933 PC A04/MF A01
National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.
Fitness-for-Service Criteria for Assessing the Significance of Fatigue Cracks in Offshore Structures,
Y. W. Cheng. Aug 85, 74p NBS/TN-1088
Also available from Supt. of Docs as SN003-003-02698-1. Sponsored by Minerals Management Service, Reston, VA.

Keywords: *Cracking(Fracturing), *Fatigue(Materials), *Offshore structures, Crack propagation, Tests, Stresses, Power spectra, Steels.

Contents: An automated fatigue crack growth rate test system; The fatigue crack growth of a ship steel in saltwater under spectrum loading; Estimation of irregularity factor from a power spectrum; Fatigue crack growth in areas of stress concentration -- Plasticity and small-crack effects; and High/low stress amplitude effects on fatigue crack growth rates of a ship steel in air and in saltwater.

501,607
PB86-138021 Not available NTIS
National Bureau of Standards, Gaithersburg, MD. Reactor Radiation Div.
Spin Dynamics of the Amorphous Invar Alloy Fe(0.86)B(0.14).
Final rept.,
J. A. Fernandez-Baca, J. W. Lynn, J. J. Rhyne, and G. E. Fish. 1985, 3p
Sponsored by National Science Foundation, Washington, DC.
Pub. in *Jnl. of Applied Physics* 57, n1 p3545-3547, 15 Apr 85.

Keywords: Iron alloys, Boron containing alloys, Neutron scattering, Invar, Reprints, *Spin waves, Amorphous materials, Heisenberg ferromagnets.

High-resolution neutron scattering studies have been made of the long wavelength spin excitations in a ribbon sample of amorphous Fe(0.86)B(0.14), which exhibits Invar properties. Spin waves were observed. The spin wave energies are well described by a dispersion relation. There are no anomalies in the spin-wave lifetimes at long wavelengths which appear to relate to the Invar effect seen in the Fe(x)B(1-x) system.

501,608
PB86-138575 Not available NTIS
National Bureau of Standards (NEL), Washington, DC. Semiconductor Materials and Processes Div.
Hot Photoluminescence in Beryllium-Doped Gallium Arsenide.
Final rept.,
E. A. Imhoff, M. I. Bell, and R. A. Forman. 1985, 4p
Pub. in *Solid State Communications* 54, n10 p845-848 1985.

Keywords: *Gallium arsenides, *Photoluminescence, Energy gap, Beryllium, Phonons, Reprints, Doped materials, Hot electrons, Molecular beam epitaxy.

Hot photoluminescence in GaAs:Be is reported for the first time. The emission from a sample with $p=6.5 \times 10^{16}$ to the 16th power/cc at 10 K consists of a shoulder at 1.803 eV followed by a series of broad peaks at 1.781, 1.742, 1.704, 1.666, and 1.628 eV. Analysis of the results supports a decay model involving hot electron-acceptor recombination and implies an L - Gamma splitting of $320 \pm$ or -4 meV in the conduction band at 0 K.

501,609
PB86-139938 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Semiconductor Materials and Processes Div.
Evidence of Lattice Relaxation in Platinum-Doped Silicon.
Final rept.,
S. Mayo, J. R. Lowney, and M. I. Bell. 1985, 10p
Pub. in *Proceedings of Materials Research Society Symposium Microscopic Identification of Electronic Defects in Semiconductors*, San Francisco, CA., April 15-18, 1985, v46 p297-306 1985.

Keywords: *Silicon, Acceptor materials, Platinum, Cross sections, Cryogenics, *Photoionization, Crystal defects, Deep levels.

The photoionization cross section of the platinum-acceptor level in silicon was measured (in relative units) as a function of photon energy. Capacitance transients due to electron emission from this level were studied in a p(+)n gated photodiode at temperatures of 40, 60, and 80 K. The results provide the first clear experimental evidence of lattice relaxation associated with a deep level in silicon.

501,610
PB86-142650 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Electroreflectance of PZT Ceramics.
Final rept.,
S. H. Shin, F. H. Pollak, and M. J. Bell. 1980, 1p
Sponsored by Office of Naval Research, Arlington, VA.
Pub. in *Ferroelectrics* 27, n1-4 p147 1980.

Keywords: Ceramics, Reprints, *Lead zirconate titanates, *Electroreflectance, Aging(Materials), Optical modulation.

Application of the technique of surface barrier electroreflectance to opaque, insulating PZT ceramics is reported. The results constitute the first observation of

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hysteresis in these materials by optical means and demonstrate the potential value of this method in studies of the switching and aging of ceramics. Asymmetric hysteresis and switching behavior is described, which is apparently related to the growth of space charge fields during aging. The time dependence of the polarization during low-field switching is shown to resemble closely that of the dielectric and piezoelectric properties during aging.

501,611
PB86-142767 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Surface Science Div.
Energy and Material Dependence of the Inelastic Mean Free Path of Low-Energy Electrons in Solids.
Final rept.,
C. J. Powell. 1985, 5p
Pub. in Jnl. of Vacuum Science and Technology A3, n3 p1338-1342 May/Jun 85.

Keywords: *Electron scattering, *Mean free path, Carbon, Magnesium, Aluminum, Aluminum oxide, Copper, Silver, Gold, Bismuth, Inelastic scattering, Reprints, EV range 100-1000, KeV range 01-10, Energy dependence.

Calculations have been made of the inelastic mean free paths (IMFP's) of 100-2000-eV electrons in C, Mg, Al, Al₂O₃, Cu, Ag, Au, and Bi. These calculations have been based on experimental optical data and on theory. The optical data gives the dependence of the differential inelastic scattering cross section at zero momentum transfer on electron energy loss; the data used here satisfy optical sum rules closely. Theory is needed to specify the dependence of the differential inelastic scattering cross section on momentum transfer; results for free-electron-like solids were assumed to be applicable to the present materials. The calculated IMFP's show significant deviations from the dependencies on electron energy and material expected from the formulas of Seah and Dench, Szajman et al., and Ashley.

501,612
PB86-167863 PC A09/MF A01
National Bureau of Standards, Gaithersburg, MD. Reactor Radiation Div.
NBS (National Bureau of Standards) Reactor: Summary of Activities July 1984 through June 1985,
F. J. Shorten. Dec 85, 178p NBS/TN-1217
See also PB83-218636.

Keywords: *Neutron beams, *Research projects, Nuclear research and test reactors, Neutron irradiation, Neutron activation analysis, Neutron diffraction, Neutron radiography, Materials tests, Crystal structure, Nondestructive tests, Molecular dynamics.

The report summarizes all those programs which depend on the NBS reactor. It covers the period from July 1984 through June 1985. 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, radiation effects studies, neutron radiography, and nondestructive evaluation.

20M. Thermodynamics

501,613
PB85-196285 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Isothermal Equations of State of H₂O-VII and D₂O-VII.
Final rept.,
R. G. Munro, S. Block, F. A. Mauer, and G. Piermarini. 1982, 5p
Pub. in Jnl. of Applied Physics 53, n9 p6174-6178 Sep 82.

Keywords: *Ice, *Lattice parameters, *Equations of state, *Bulk modulus, Heavy water, Deuterium compounds, Reprints, Pressure dependence.

Lattice parameters and cell volumes at room temperature are reported for H₂O-VII to 36 GPa and for D₂O-VII to 32 GPa. The data are fitted to seven isothermal equations of state from which are derived averaged values of the isothermal bulk moduli and their pressure

derivatives as a function of pressure. The procedures employed for treating the data and the reliability of the derived results are assessed for both materials.

501,614
PB85-197739 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Critical Correlations and the Square-Gradient Theory.
Final rept.,
R. F. Kayser, and H. J. Raveche. 1983, 4p
Pub. in Physical Review Letters 50, n5 p298-301, 31 Jan 83.

Keywords: *Fluids, *Critical point, Nonlinear differential equations, Reprints, Correlation functions.

A nonlinear differential equation for the asymptotic decay of the pair correlation function of a fluid at its critical point is obtained from the square-gradient theory (and its extension to fourth-order), and analyzed when the critical exponent η is either zero or nonzero. Its solutions are shown to be consistent with the correct power-law decay if and only if the ordinary scaling relations together with hyperscaling (for $\eta > 0$) are valid.

501,615
PB86-142791 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Thermal Processes Div.
Measurement of Thermal Radiation Properties of Materials.
Final rept.,
J. C. Richmond. 1980, 27p
Pub. in Proceedings of the European Thermophysical Properties Conference (6th), Dubrovnik, Yugoslavia, June 26-30, 1980, High Temperature-High Pressures 11, n4 p355-381.

Keywords: *Thermal radiation, Reflectance, Absorbance, Emittance, Transmittance, Blackbody radiation, Calorimetry, Radiometry.

The thermal radiation properties, reflectance, absorbance, emittance and transmittance, are defined, and the equations showed the relationships between these properties are given. The equations relating the amount and the spectral and geometric distribution of the flux emitted by a blackbody or complete radiator to its temperature are given, and it is shown how these equations can be applied to a real material by use of thermal radiation properties of the solid materials are briefly described and illustrated, and references are given to the original papers describing such measurements.

21.

PROPULSION AND FUELS

21B. Combustion and Ignition

501,616
PB85-177988 PC A04/MF A01
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.
Effect of Wall and Room Surfaces on the Rates of Heat, Smoke, and Carbon Monoxide Production in a Park Lodging Bedroom Fire,
B. T. Lee. Feb 85, 57p NBSIR-85/2998
Sponsored by National Park Service, Washington, DC.

Keywords: *Buildings, *Furnishings, *Fire tests, *Heat flux, Flashover, Burning rate.

A furnishing arrangement representative of those in U.S. Park Service lodging facilities was evaluated for its open burn (free burn) characteristics. The arrange-

ment consisted of a double bed with a wood headboard and one wood night table. The proximity of a wall and the effect of a room on the combustion of the same arrangement were examined. Wall finish materials were gypsum board and plywood. The presence or combustibility of an adjacent wall did not have a significant effect on the burning behavior of the furnishing arrangement. Nor did the effect of a room enclosure for the first few minutes subsequent to ignition. However, after this initial time interval, the effect of a room, lined with gypsum board finish, on the burning furnishings was pronounced, with flashover occurring as early as 233 s with heat release rates of over 2 MW. This compared with a peak rate of 1.2 MW for the open burn. Wood paneling in the room increased the peak rate to 7 MW. Mass flow of hot gases, smoke, and carbon monoxide from the room fires were measured. The use of a sprinkler or automatic door closing device activated by a smoke detector was shown to prevent room flashover.

501,617
PB85-178002 PC A02/MF A01
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.
Significant Parameters for Predicting Flame Spread,
J. G. Quintiere. Feb 85, 13p NBSIR-85/3109

Keywords: *Flame propagation, Equations, Combustion, Predictions, Flammability, Walls, Vents, Enclosures, Temperature, Room fires.

Flame spread is considered on a vertical wall surface in a vented enclosure. A theoretical formulation is developed to describe the burning and fire spread behavior and its response to the changing environmental conditions of the room. These formulations have been kept simple in form, but consistent with current levels of accuracy and completeness. The primary aim was to establish the relevant and significant set of dimensionless parameters which govern the fire spread process. These are given in terms of room geometric factors and wall flammability properties. No solution of the equations has been developed.

501,618
PB85-178101 PC A06/MF A01
Brown Univ., Providence, RI. Div. of Engineering.
Experimental Study of the Burning of Pure and Fire Retarded Cellulose.
Doctoral thesis,
S. S. Tewari. Jan 85, 104p NBS/GCR-85/485
Grant NB83-NADA-4017

Keywords: *Cellulose, *Burning rate, *Fire resistant coatings, *Flammability testing, *Cellular materials, Combustion, Sodium hydroxide, Sodium carbonates, Samples, Pyrolysis, Wood, Surface temperature, Theses, Experimental design, Char, Oxygen, Concentration(Composition).

The burning of charring materials is studied using samples prepared from pure cellulose and the cellulose which has been fire retarded by the addition of Sodium Hydroxide and Sodium Carbonate. The samples which are hemispherically nosed cylinders, are burned in a vertical orientation in a variable oxygen/nitrogen mixture at atmospheric pressure. Ambient oxygen concentration has a stronger effect on the change in burning rate and surface temperature than a proportional change in the retardant concentration. This dominant effect of oxygen concentration is also evident in a significant increase in the amount of retardant needed to cause extinction (both stagnation point and flaming) as the ambient oxygen concentration is increased. At sufficiently high oxygen concentration no extinction is found for the maximum retardant concentration used in this study. A practical consequence of these findings is the need to exercise proper caution in using these retardants in cellulosic products in oxygen rich environments.

501,619
PB85-182723 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Quasichemical Melt Polymerization Model of SEED/SLAG Interaction.
Final rept.,
L. P. Cook. 1980, 8p
Sponsored by United Nations Educational, Scientific and Cultural Organization, Paris (France), and Department of Energy, Washington, DC.

Pub. in Proceedings of International Conference on MHD Electrical Power Generation (7th), Cambridge, MA., June 16-20, 1980, v1 p212-219.

Keywords: *Mathematical models, *Slags, *Magneto-hydrodynamics, *Combustion, *Melts, Experimental design, Potassium carbonates, Oxidation, *Quasichemistry, *Seed-slag interactions, Phase equilibrium, Aluminum potassium silicates.

Experimental data illustrating KAlSiO₄/melt interaction as a function of temperature are presented for synthetic channel slags modeling MHD combustion of 'Eastern' and 'Western' coals. The phase equilibrium behavior of the two slags is markedly different. In particular, a wide area of high temperature liquid immiscibility is found in the iron rich 'Eastern' slag. However the quasichemical model, by choice of appropriate parameters, can be used to fit the two-liquid data for the 'Eastern' slag. The quasichemical model suggests a sensitive relation between oxidation state and melt phase equilibrium behavior. The need for quantitative data on the effect of Fe(+3) on melt polymerization is discussed.

501,620
PB85-187599 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Predictions of Pressure and Composition Limits for Confined Hydrogen-Oxygen Detonations.

Final rept.,
H. G. Semerjian, and J. E. Dove. 1981, 6p
Sponsored by Combustion Inst., Bordeaux (France). France Section.
Pub. in Proceedings of Int. Specialists Meeting of the Combustion Institute (1st), Bordeaux, France, July 20-25, 1981, p455-460.

Keywords: *Detonation waves, *Boundary layers, *Combustion, *Reaction kinetics, Pressure, Mathematical models.

Pressure and composition limits, and velocity deficits have been calculated for confined hydrogen-oxygen detonations, and the effect of initial pressure, mixture composition and tube diameter on detonability limits has been investigated. A quasi-one-dimensional Zel'dovich-von-Neumann-Doring model is used to represent the reaction zone, and the effect of the viscous boundary layer along the wall is accounted for using a negative displacement thickness. The model predicts all the experimentally observed features of detonation waves; (a) all confined detonation waves travel at a velocity somewhat lower than the C-J velocity, and the velocity deficit is dependent on pressure, gas composition and tube diameter; (b) detonability limits exist and again depend on pressure, composition and tube diameter. Effect of the chemical reaction scheme and multidimensional effects are also discussed.

501,621
PB85-189298 Not available NTIS
National Bureau of Standards (NEL), Washington, DC.
Center for Fire Research.

Heating Rates in Fire Experiments.
Final rept.,
C. Huggett. Aug 84, 3p
Pub. in Jnl. of Fire Sciences 2, p257-259 Jul/Aug 84.

Keywords: *Fire tests, Heating, Combustion, Experimentation, Simulation, Reprints, Solid fuels.

The rate at which a solid fuel sample should be heated in a small scale experiment to best simulate conditions in a real fire is a subject of continuing discussion.

501,622
PB85-196137 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
High Speed Three-Dimensional Diagnostics in Combustion.

Final rept.,
R. Goulard, P. J. Emmerman, R. J. Santoro, and H. G. Semerjian. 1982, 10p
Sponsored by National Academy of Engineering, Washington, DC., and Chinese Scientific and Technical Association, Beijing.
Pub. in Proceedings of the U.S.-China Conference on Energy (1st), Beijing, China, November 7-12, 1982, p162-171.

Keywords: *Combustion, Temperature, Concentration(Composition), *Optical tomography.

Recent research in turbulent combustion has shown the important role played by coherent structures in the

onset of complete reactants mixing. An understanding of their three dimensional, time-histories would be an essential step into better combustor design and the study of turbulence fundamentals. A new diagnostics technique - optical tomography - is described, with its capability for high speed, three-dimensional resolution of temperature and concentrations.

501,623
PB85-197671 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Enthalpy of Combustion of Adenine.

Final rept.,
D. R. Kirklin, and E. S. Domalski. 1983, 7p
Pub. in Jnl. of Chemical Thermodynamics 15, n10 p941-947 1983.

Keywords: *Adenine, *Enthalpy, *Combustion tests, Thermodynamic properties, Nucleotides, Heat of formation, Heat measurement, Reprints.

The enthalpy of combustion for a commercial adenine sample of 99.9 percent purity was measured in an an-eroid adiabatic bomb calorimeter. The enthalpy of combustion at 298.15 K for the reaction.

501,624
PB85-200202 PC A08/MF A01
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.

Summaries of Center for Fire Research (of the National Bureau of Standards) Grants and In-House Programs - 1984.

Final rept.,
S. M. Cherry. Apr 85, 162p NBSIR-85/3136
See also PB84-155340.

Keywords: *Fires, Fire protection, Combustion, Evacuating(Transportation), Flame propagation, Fire safety, Smoke, Soot, Toxicity, Polymers, *Fire research, Computer applications.

This report was prepared for distribution at the 1984 Annual Conference on Fire Research, October 17-19, 1984. It contains extended abstracts of grants and contracts for fire research sponsored by the Center for Fire Research, National Bureau of Standards, as well as descriptions of the internal programs of the Center for Fire Research.

501,625
PB85-202745 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Fire Safety Technology Div.

Calculations of Three Dimensional Buoyant Plumes in Enclosures.

Final rept.,
H. R. Baum, and R. G. Rehm. 1984, 23p
Pub. in Jnl. of Combustion Science and Technology 40, n1-4 p55-77 1984.

Keywords: *Plumes, *Combustion, Enclosures, Convection, Fires, Mathematical models, Aerosols, Fluid flow, Eddies, Reprints.

A computational model of the three dimensional buoyant convection and aerosol dynamics induced by a weak volumetric source of heat and mass is presented. The hydrodynamics is directly based on the time dependent inviscid Boussinesq equations. No turbulence model or other empirical parameters are introduced. The use of Lagrangian particle tracking together with an exact solution of the Smoluchowski equation allows prediction of smoke aerosol transport and coagulation. The combined calculations represent predictions involving five independent variables. Flow features from three different configurations are illustrated with both Eulerian and Lagrangian displays of information. Sample aerosol coagulation results are compared with data from a wood fire. The computer resources required are discussed and an assessment of the current feasibility of large-eddy simulations in fire research is made.

501,626
PB85-202778 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Office of Fire Research Resources.

Workshop on Flame Radiation and Soot. Proceedings: Ad Hoc Mathematical Fire Modeling Working Group.

Final rept.,
R. S. Levine. Feb 85, 18p
Pub. in Jnl. of Fire Technology 21, n1 p41-58 Feb 85.

Keywords: *Flame propagation, *Fire extinguishing agents, Soot, Heat transfer, Combustion, Fires, Reprints, Fire models.

From the several research projects on extinguishment, that there are two important extinguishment mechanisms, and both of them can be incorporated into the models: Method 1 requires enough extinguishing agent so that its heat of vaporization is of the order of the heat stored in the ceiling layer plus the thermal output of the fire. It is possible that the stirring caused by a sprinkler in a small room will rapidly carry vaporized extinguishing agent into the lower layer. Method 2 requires only a few percent of the amount of extinguishing agent in method 1, provided it can be efficiently delivered to the fuel surface.

501,627
PB85-203487 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.

Smoke Measurements: An Assessment of Correlations between Laboratory and Full-Scale Experiments.

Final rept.,
J. G. Quintiere. 1982, 16p
Pub. in Fire and Materials 6, n3-4, p145-160 Sep-Dec 82.

Keywords: *Smoke, *Fires, Measurement, Correlations, Tests, Light transmission, Visual perception, Visibility, Equations, Reprints.

An extensive review is presented demonstrating the nature of comparison between full-scale fire smoke data and test method results for materials. These correlations are presented in terms of consistent parameters established through a development of the governing equations for smoke concentration and light attenuation. Visibility data pertaining to light transmission through smoke is presented. Recommendations are made for further research to establish a sounder basis for correlations, and a practical strategy is suggested for proceeding in the present.

501,628
PB85-205177 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Fire Safety Technology Div.

Wall Flames and Implications for Upward Flame Spread.

Final rept.,
J. Quintiere, M. Harkleroad, and Y. Hasemi. 1985, 16p
Pub. in Proceedings of AIAA (American Institute of Aeronautics and Astronautics) Aerospace Sciences Meeting (23rd), Reno, Nevada, January 14-17, 1985, AIAA-85-0456, 16p 1985.

Keywords: *Flame propagation, Polyurethane resins, Fires, Aircraft, Foam, Combustion, Heat transfer, Polymethyl methacrylate, Particle boards, Wool, Nylon, Flammability, *Flame spread tests.

The study marks the second phase of a project aimed at developing a predictive and quantitative measurement strategy for flame spread on materials. It deals with the heat transfer processes important to the inception of upward flame spread. In the study, six materials have been consistently used throughout. They included: polymethylmethacrylate (PMMA); Douglas fir particle board; low density rigid polyurethane foam (GM-31); flexible polyurethane foam; wool/nylon carpet and an aircraft interior panel. Vertical sections of the materials, nominally 28 x 28 cm were irradiated by infrared heaters and burned. Flame height and the heat transfer to a cool (60 degrees C) vertical copper plate were dynamically recorded. The results are analyzed in terms of the flame height and the energy release rate of the wall fire.

501,629
PB85-205235 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Fire Safety Technology Div.

Finite Difference Solutions for Internal Waves in Enclosures.

Final rept.,
H. R. Baum, and R. G. Rehm. Dec 84, 20p
Pub. in SIAM (Society for Industrial and Applied Mathematics) Jnl. on Scientific and Statistical Computing 5, n4 p958-977 Dec 84.

Keywords: *Finite difference theory, *Fluid flow, *Internal waves, *Enclosures, Partial differential equa-

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Group 21B—Combustion and Ignition

tions, Buoyancy, Computation, Fires, Stratification, Stability, Reprints.

Finite difference approximations to the set of partial differential equations governing internal waves are investigated. Analytical solutions describing waves in an enclosure in two and three dimensions are obtained. The schemes considered are second order accurate in space and include first order explicit and second order time differencing. The solutions are used to investigate the temporal stability and long term accuracy of all schemes. The mode frequencies and wave shapes obtained from each difference scheme are compared with the solutions both to the corresponding partial differential equations and to equations obtained by discretizing in space only. The solutions have been used by the authors to help develop a finite difference code designed to compute non-linear buoyancy-driven flows of the type that arise in enclosure fires.

501,630

PB85-205276 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Fire Safety Technology Div.
Perspective on Compartment Fire Growth.
Final rept.,
J. Quintiere. 1984, 44p
Pub. in Combustion Science and Technology 39, n1-6 p11-54 1984.

Keywords: *Fires, Flame propagation, Combustion, Heat transfer, Fluid mechanics, Reprints, *Compartment fires, *Fire growth.

A review was made of research related to fire growth in compartments. Mention is made of the zone and field model approaches that have been used to describe many aspects of compartment developing fires. Primarily the review is organized by phenomena associated with compartment fires. These include fluid mechanic, heat transfer and combustion processes. Each phenomenon is discussed and work is presented to illustrate predictive techniques. Limitations and deficiencies in the authors understanding are discussed. A previously unavailable analysis of radiative transfer in an enclosure for a two layer participating gas is also presented.

501,631

PB85-205672 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Structure and Equilibria of Polyaromatic Flame Ions.
Final rept.,
S. E. Stein. 1983, 8p
Pub. in Combustion and Flame 51, n3 p357-364 1983.

Keywords: *Molecular structure, *Aromatic polycyclic hydrocarbons, *Ions, *Reaction kinetics, *Flammability testing, *Thermodynamics, High temperature tests, Experimental design, Sampling, Stability, Reprints.

The aim of this work is to determine structures of a series of major hydrocarbon ions found in the burnt gas region of fuel-rich acetylene flames. Both kinetic and thermodynamic arguments are presented to first show that protonated and ionized benzenoid polynuclear aromatics are more stable than any of their non-benzenoid structural isomers, and then that the ionized forms are expected to predominate in low pressure flames above about 1600 K. The fact that only the protonated forms are detected in flame-sampling experiments is attributed to rapid H-atom addition reactions in a region cooled by the sampling probe. This work demonstrates the utility of thermokinetic estimation methods for determining the most stable ion structures, correcting for sampling effects and finding ion reaction pathways.

501,632

PB85-205680 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Laser Spectroscopy - Multiphoton Techniques Expand Combustion Diagnostic Capabilities.
Final rept.,
K. C. Smyth. 1983, 2p
Pub. in Nature 301, n5900 p467-468 Feb 83.

Keywords: *Combustion, *Photons, *Ionization, *Fluorescence, *Flammability testing, Reprints, *Laser spectroscopy.

The application and future prospects of multiphoton ionization and multiphoton fluorescence experiments to flame diagnostics are described.

501,633

PB85-205698 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Soot Particle Measurements in Diffusion Flames.
Final rept.,
R. J. Santoro, H. G. Semerjian, and R. A. Dobbins. 1983, 16p
Pub. in Combustion and Flame 51, n2 p203-218 1983.

Keywords: *Soot, *Particle size, *Combustion, *Flames, Chemical reactions, Fluorescence, Oxidation, Light scattering, Ethane, Diffusion, Reprints.

The formation and growth of soot particles in a co-anular diffusion flame has been studied using a laser extinction/scattering technique for particle size measurement. Measurements have been obtained with ethene as the fuel for various fuel flow rates. The results reveal that the flame can be broadly divided into two regions. One characterized as a region of growth where soot formation processes dominate and a second in which oxidation processes are dominant. Measurement show that soot is first observed to form low in the flame in an annular region inside the main reaction zone. At higher locations this annular region widens until the entire flame is observed to contain particles. Measurements of depolarized scattered light and fluorescence have also been obtained and indicate a correlation between the species responsible for these processes and soot growth. Results indicate that the particle formation region obeys closely the Burke Schumann analysis for flow rate dependence, where as substantial differences occur in the oxidation region. Measurements have also been obtained using ethane as the fuel as an initial comparison of fuel structure effects.

501,634

PB85-207405 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Simon H. Ingberg -- Pioneer in Fire Research.
Final rept.,
A. F. Robertson. Feb 85, 4p
Pub. in ASTM (American Society for Testing and Materials) Standardization News 13, n2 p50-53 Feb 85.

Keywords: *Research projects, *Fire tests, Safety, Construction materials, Buildings, Reprints, *Simon H. Ingberg.

Ingberg's work is recognized, respected, and studied not only in the United States but in every nation that tries to make progress in control of unwanted fires.

501,635

PB85-208049 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Fire Safety Technology Div.
Approach to Hazard Assessment of Combustion Products in Building Fires.
Final rept.,
A. J. Fowell. 1984, 12p
Pub. in Proceedings of Flame Retardancy Advances in Fire Safety: Regulations, Testing, Product, Markets, Pine Mountain, GA., March 28-30, 1984, p24-35.

Keywords: *Fire tests, *Toxicity, *Combustion products, *Materials tests, *Building codes, Assessments, Air pollution, Hazards, Smoke, Burning rate, Predictions, *Air pollution effects (Humans), *Indoor air pollution.

A framework for addressing hazards associated with the spread of smoke and hot gases from fires in buildings is proposed, and the current predictive capabilities for each component of that framework are described. A method for assessing the significance of the toxicity of the combustion products of a material in relation to its other fire properties is proposed.

501,636

PB85-208130 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.
Bench-Scale Methods for Prediction of Full-Scale Fire Behavior of Furnishings and Wall Linings.
Final rept.,
V. Babrauskas. 1984, 26p
Pub. in SFPE (Society of Fire Protection Engineers) Technology Report 84-10, p1-25 1984.

Keywords: *Furniture, *Walls, *Linings, Flammability, Measurement, Flashover, Fires, Heat transfer, Flame propagation, Test equipment, Ignition, Fire resistant materials, Reprints, *Fire tests.

Fire development in a room involves three basic phenomena: ignition, flame spread, and heat release rate. Of these, the heat release rate tends to be more important than the other two in most common fire scenarios. Heat release rates are difficult to determine accurately by direct, sensible-enthalpy measurements. It has recently been used in two test apparatuses developed at the National Bureau of Standards: a furniture calorimeter for conducting full-scale tests, and a cone calorimeter for conducting bench-scale tests. Bench-scale data have now been gathered on upholstered furniture and on wall-lining materials, with corresponding full-scale data available from furniture calorimeter or room fire measurements. In both cases, bench-scale measurements allowed the successful prediction of full-scale data for variables of interest, which were the peak rate of heat release and the time to flashover.

501,637

PB85-208502 PC A02/MF A01
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.
Fire Research Publications, 1984.
Final rept.,
N. H. Jason. May 85, 20p NBSIR-85/3153
See also PB84-217066.

Keywords: *Fires, Bibliographies, Combustion, Smoke, Toxicity, Fire safety, Fire protection, Meetings, *Fire research, Means of degrees.

Fire Research Publications, 1984 is a supplement to previous editions; the last five editions are referenced below. Information about earlier editions is available upon request. 1979--NBSIR 80-2114, PB80-103335; 1980--NBSIR 81-2272, PB81-203317; 1981--NBSIR 82-2499, PB82-220104; 1982--NBSIR 83-2706, PB83-238915; 1983--NBSIR 84-2871, PB84-217066. In a departure from the authors usual practice of citing only publications prepared by the Center for Fire Research (CFR) staff, by other National Bureau of Standards (NBS) personnel for CFR, or by external laboratories under contract or grant from the CFR, they are pleased to include the papers presented at the Howard Emmons' Conference, Fire Science for Safety. The CFR devoted its 1983 Annual Conference to invited papers on subject areas that have been significantly influenced by Professor Emmons and his students. The Conference was held at NBS in Gaithersburg, MD, August 23-24, 1983. Selected papers have been published in a special issue of Combustion Science and Technology, Vol. 39-40, 1984 and are cited herein.

501,638

PB85-224483 PC A04/MF A01
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.
Evaluation and Refinement of Test Methods Used for Measuring Fire Hazards of Shipboard Hull Insulations and Mattress Insert Foams.
B. T. Lee. May 85, 57p NBSIR-85/3148
Sponsored by Naval Sea Systems Command, Washington, DC.

Keywords: *Fire tests, *Construction materials, *Insulation, *Ship hulls, *Bedding equipment, Smoke, Carbon monoxide, Foam, Heat transmission, Burning rate, Experimental design, Fire hazards, Laboratory equipment, Polyphosphazene.

A quarter-scale room fire test developed at NBS was used to help develop a preliminary approach for fire hazard assessment of wall-ceiling combinations of hull insulation materials. The quarter-scale test has been refined to include measurement of heat release rate, smoke, and carbon monoxide. In addition, polyphosphazene foam insulations were evaluated with this test. The quarter-scale test was also modified for testing mattress insert materials, including polyphosphazene foam. Existing tests, used for measuring total heat, rate of heat release, and smoke production, were also used to evaluate these materials. Heat release rate measurements with the Ohio State University apparatus and smoke measurements with the ASTM E 662 test, modified for horizontal placement of specimens, gave adequate evaluation of the fire hazards of mattress insert materials.

501,639

PB85-226520 PC A06/MF A01
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.

Products of Wood Gasification,
T. J. Ohlemiller, T. Kashiwagi, and K. Werner. Apr
85, 115p NBSIR-85/3127
Sponsored by Department of Energy, Washington, DC.

Keywords: *Stoves, *Gasification, *Air pollution, *Pyrolysis, *Wood, Combustion products, Gas chromatography, Chromatographic analysis, Heating equipment, Residential buildings, Gas analysis, Thermal degradation, *Wood burning appliances, *Air pollution detection, Path of pollutants, Solid wastes.

The increasing problem of pollution from wood-burning stoves has prompted this examination of the basic gasification process of wood under conditions encompassing those in stoves. Other variables were sample grain orientation, thickness, exposure time and moisture content. Sample weight was followed in some tests; sample temperature (5 thermocouples) was followed in others. In all tests, all evolved products were either monitored (H₂O, CO, CO₂, total hydrocarbons not condensable at -40C) or trapped and analyzed (condensable organic species) by gas chromatography and mass spectroscopy. Chromatographic fingerprints of the organic condensate indicated that its composition does not vary a great deal for the conditions examined here. The fingerprints from the radiative heating tests bear a strong resemblance to those of the smoke condensate from a wood stove.

501,640
PB85-246080 PC A04/MF A01
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.
Polyesters: A Review of the Literature on Products of Combustion and Toxicity,
E. Braun, and B. C. Levin. Jan 85, 72p NBSIR-85/3139
Sponsored by Consumer Product Safety Commission, Washington, DC.

Keywords: *Polyester resins, *Combustion products, *Toxicity, *Pyrolysis, *Fire tests, *Thermoplastics, Reviews, Textiles, Construction materials, Fire resistant materials, Air pollution, Plastics, Additives, *Indoor air pollution, Consumer products.

The available literature was reviewed to determine the nature and extent of information available on the thermal decomposition products and the toxicity of the combustion products of polyester materials used in consumer applications such as textiles and construction. The literature review is limited to the publications printed in English through June, 1984. The thermal decomposition products of polyesters are a function of temperature and oxygen content of the atmosphere. In general, as the temperature increases, the quantity of heavier hydrocarbons decreases and the production of CO and CO₂ increases. The presence of flame retarded additives, such as bromine and chlorine containing compounds, product halogenated combustion products. The use of phosphorus and bromine together in the same flame retardant finish increases the concentration of low molecular weight compounds. Thirteen different test protocols have been used to evaluate the toxicity of various types of polyester. In general, the results from large-scale tests are ambiguous because of the presence of other materials in addition to the polyesters.

501,641
PB85-248755 PC A08/MF A01
California Inst. of Tech., Pasadena. Div. of Engineering and Applied Science.
Experimental Study of Environment and Heat Transfer in a Room Fire. Mixing in Doorway Flows and Entrainment in Fire Plumes.
Rept. for 1982-84,
E. E. Zukoski, T. Kubota, and C. S. Lim. May 85,
175p NBS/GCR-85/493
Grant NB82-NADA-3033

Keywords: *Fire tests, *Heat transfer, *Building fires, *Combustion products, Plumes, Experimental design, Doors, Ceilings(Architecture), Gravity, Experimental design, Concentration(Composition), Mixing, Mathematical models, Gas flow.

The report contains a description of an ongoing study of gravity currents for conditions which match those the authors expect to find in unwanted fires in buildings. A review is made of the pertinent literature and a description is given of the flow regimes which can exist for ideal gravity currents when viscous effects, heat transfer, and mixing are ignored. The influence of boundary conditions fixed by the method used to with-

draw the fluid displaced by the current is given. Algebraic equations for the thickness of the current and the velocity of the head are derived for these ideal flows. The influences of viscosity and mixing are briefly discussed and the status of salt water and gas modeling experiments is given.

501,642
PB86-102233 PC A04/MF A01
Pennsylvania State Univ., University Park. Dept. of Mechanical Engineering.
Investigation of Turbulent Fires on Vertical Walls: Wall Plume Structure,
M. C. Lai, S. M. Jeng, and G. M. Faeth. Feb 85, 74p
NBS/GCR-85/486
Grant NB81-NADA-2044

Keywords: *Fires, Air flow, Turbulence, Walls, Flow visualization, Measurement, Combustion, Flames, *Wall flow, Buoyant plume, Fire plume.

A theoretical and experimental study designed to improve understanding of buoyant fires is described. The main objective is to study turbulent fires along surfaces, however, several noncombusting and combust-ing flow configurations, which offer opportunities to highlight aspects of this problem under simpler circumstances, were considered during the work, e.g., buoyant noncombusting wall plumes, for studies of flow properties; and turbulent round flames, for studies of flame radiation properties. Various phases of the study are reported separately; this report considers results for noncombusting wall plumes.

501,643
PB86-102266 PC A03/MF A01
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.
Pyrolysis of Cellulose, an Introduction to the Literature,
T. Hirata. Aug 85, 36p NBSIR-85/3218

Keywords: *Cellulose, *Pyrolysis, *Bibliographies, *Fire resistant materials, *Biomass, Reaction kinetics, Molecular structure, Mathematical models, Polymerization, Fine structure, Chemical properties, Wood, Anaerobic processes.

Topics related to cellulose pyrolysis are briefly surveyed under several headings. The principal aim is to give the reader some grasp of the issues involved and provide a guide to the relevant literature; 171 references are cited. The headings include: Changes in cellulose fine structure with heating; chemical changes during pyrolytic weight loss and kinetic modeling of pyrolysis. Principal emphasis is on the last area; it is concluded that no current model adequately predicts both the observed changes in degree of polymerization and the weight loss during heating.

501,644
PB86-108347 PC A03/MF A01
Notre Dame Univ., IN. Dept. of Aerospace and Mechanical Engineering.
Scaling Parameters of Flashover.
Final rept.,
A. M. Kanury. Jul 85, 50p NBS/GCR-85/497
Contract NB83-NADA-4018
Sponsored by National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.

Keywords: *Flashover, *Fires, Combustion, Walls, Flames, Flame propagation, Scaling, Room fires, Fire growth, Compartment fires.

The topic of concern in this project is room fire growth to flashover. The objective is to develop scaling rules for flashover time and to apply these rules to certain existing room fire flashover test data. In this report, the scaling rules are deduced from first principles of energy and mass conservation describing the physics of fire growth. The nondimensional scaling parameters are all obtained in the desirable terms of fundamental combustion properties. Collection, estimation, and deduction of these fundamental properties for the materials involved in the concerned fire tests has to be done in the immediate future to evaluate the scaling parameters for correlating the test data.

501,645
PB86-110004 PC A04/MF A01
Factory Mutual Research Corp., Norwood, MA.

Scale Effects on Fire Properties of Materials,
A. Tewarson. Feb 85, 52p NBS/GCR-85/488
Grant NB83-NADA-4021
Sponsored by National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.

Keywords: *Materials tests, *Flammability testing, Experimental design, Plastics, Wood, Pyrolysis, Paper, Cellulose, Carbon monoxide, Furniture, *Indoor air pollution, *Toxic substances.

The objective of this study was to examine the scale effects on fire properties of materials over a range of fire sizes from 10 kW to 5000 kW-scale fires. Experiments were performed for cellulosic materials, alone and in combination with synthetic materials in box-like and crib-like configurations. Experimental results for a pool-like material configuration from our previous study and for enclosure fires of wood cribs reported in the literature were also used. For turbulent fires of various sizes with various geometrical material configurations, a chemical similarity was found for each material for each specified value of the ventilation parameter. The decomposition mode in the combustion of the cellulosic material was found to be very important for CO and particulates, but less important for CO₂ and heat.

501,646
PB86-111986 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Fire Safety Technology Div.
Two Approaches to the Analysis of Actual Fires.
Final rept.,
J. A. Rockett. 1985, 12p
Pub. in Fire Safety Jnl. 9, p17-28 1985.

Keywords: *Fire tests, Reprints, Numerical solution.

Two calculations are described. One used only simple algebra to show the rate of development of a critical aspect of a fire. The other used one of our most elaborate computer based schemes to extend the results of full-scale fire tests to additional, important situations. Both provided useful results. The significance of this is that it is not the complexity of a calculation that is important but its relevance to the problem at hand.

501,647
PB86-112364 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Fire Safety Technology Div.
Computer Modeling for Smoke Control Design.
Final rept.,
J. H. Klote. 1985, 8p
Pub. in Fire Safety Jnl. 9, p181-188 1985.

Keywords: *Building codes, *Fire safety, *Mathematical models, *Smoke abatement, Ventilation, Design criteria, Pressure, Reprints, *Indoor air pollution, Computer applications, Numerical solution.

The concept of using pressurization to control smoke movement in building fire situations has developed considerably over the past decade and a half. This paper discusses a steady state, network, airflow computer model which can be used for smoke control system design. Assumptions, equations and numerical solution technique are presented. An example problem also is included.

501,648
PB86-114022 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.
Study of the Radiative Ignition Mechanism of a Liquid Fuel Using High Speed Holographic Interferometry.
Final rept.,
T. Kashiwagi, and T. Kashiwagi. 1982, 11p
Sponsored by Combustion Inst., Pittsburgh, PA.
Pub. in Proceedings of Symposium on Combustion (19th), Haifa, Israel, August 8-13, 1982, p1511-1521.

Keywords: *Ignition, *Fuels, Combustion, Experimental design, Plumes, *Interferometric halography, *Chemical reaction mechanisms, Laser applications.

The ignition mechanism of 1-decene is investigated experimentally using a high speed two-wavelength holographic interferometry technique with a framing speed of 500 f/sec for measurements of temperature and fuel vapor concentration distributions in the gas phase near the liquid surface from the CO₂ laser irradiation up to ignition. The effects of oxygen concentration using three different environments of nitrogen, air

Field 21—PROPULSION AND FUELS

Group 21B—Combustion and Ignition

and 40% O₂/60% N₂ and of peak laser flux at 260, 520 and 780 W/sq cm on the growth of the fuel vapor plume, the location of ignition and distributions of temperature and fuel vapor concentration are studied.

501,649
PB86-122975 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Thermal Processes Div.

Laser Tomography for Diagnostics in Reacting Flows.

Final rept.,
H. G. Semerjian, S. R. Ray, and R. J. Santoro. 1982, 9p
Pub. in Proceedings of AIAA/ASME Joint Thermophysics, Fluids, Plasma and Heat Transfer Conference (3rd), St. Louis, MO., June 7-11, 1982, p1-9.

Keywords: *Absorption spectra, *Flames, *Fuel air ratio, Methane, Concentration(Composition), Temperature, *Laser spectroscopy, *Tomography, Hydroxyl radical.

The laser tomography technique has been developed for simultaneous measurement of temperature and species concentration in reacting flows. Laser tomography is a multiangular absorption technique which involves making absorption measurements along M parallel rays at N equally spaced angles. These MxN measurements are then used to reconstruct the spatially resolved two-dimensional property field. Results of a simulation study are presented for a methane/air diffusion flame. Two techniques, a two-line ratio and a spectral line profile technique, have been used to obtain the temperature and OH concentration and temperature fields can be reconstructed with a resolution of better than 1%. Sensitivity of the technique to the choice of particular spectral lines, and the effect of large temperature gradients are also discussed.

501,650
PB86-122983 Not available NTIS
National Bureau of Standards (NEL), Gaithersburg, MD. Thermal Processes Div.

Laser Tomography for Temperature Measurements in Flames.

Final rept.,
H. G. Semerjian, R. J. Santoro, P. J. Emmerman, and R. Goulard. 1982, 11p
Sponsored by American Inst. of Physics, New York, and Instrument Society of America, Pittsburgh, PA.
Pub. in Proceedings of International Symposium on Temperature: Its Measurement and Control in Science and Industry (6th), Washington, DC., March 15, 1982, v5 pt1 p649-659.

Keywords: *Absorption spectra, *Flames, *Fuel air ratio, Methane, Temperature, Concentration(Composition), *Laser spectroscopy, *Tomography.

The laser tomography technique has been used for composition measurements in a laminar methane/air diffusion flame. A simulation study has also been carried out to extend the technique for simultaneous temperature and composition measurements using two-line absorption and tomographic reconstruction techniques. Laser tomography is a multiangular absorption technique which involves making M line-of-sight absorption measurements (projections) at N angles. These MxN measurements are then used to reconstruct the original two dimensional property field. These studies have demonstrated the feasibility of extending the laser tomography technique for simultaneous temperature and concentration measurements in nonuniform and nonsymmetric flow fields.

501,651
PB86-153772 PC A04/MF A01
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.
Acrylonitrile-Butadiene-Styrene Copolymers (ABS): Pyrolysis and Combustion Products and Their Toxicity - A Review of the Literature,
J. V. Rutkowski, and B. C. Levin. Dec 85, 60p
NBSIR-85/3248
Sponsored by Consumer Product Safety Commission, Bethesda, MD.

Keywords: *ABS resins, *Pyrolysis, *Combustion products, *Toxicity, *Carbon monoxide, *Hydrogen cyanide, Reviews, Plastics, Copolymers, Exposure, Polymers, Flammability testing, Oxidation, Households, Aircraft, Automobiles, Public health, Air pollution, Chemical properties, Chemical analysis, Laboratory equip-

ment, *Indoor air pollution, *Toxic substances, Consumer products.

A review of the literature was undertaken to ascertain the current knowledge of the nature of the thermal decomposition products generated from ABS and the toxicity of these evolved products into. The literature review encompasses English language publications available through June 1984. This literature surveyed showed that the principal ABS thermooxidative degradation products of toxicologic importance are carbon monoxide and hydrogen cyanide. The experimental generation of these and other volatile products is principally dependent upon the combustion conditions and the formulation of the plastic. The toxicity of ABS thermal degradation products has been evaluated by five methods. The toxicity of ABS degradation products was found to be comparable to the toxicity of the thermal decomposition products of other common polymeric materials.

501,652
PB86-166592 PC A03/MF A01
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.
Program for the Development of a Benchmark Compartment Fire Model Computer Code,
L. Y. Cooper, J. A. Rockett, H. E. Miller, and D. W. Stroup. Oct 85, 30p NBSIR-85/3252

Keywords: *Fires, *Fire safety, Fire tests, *Compartment fires, Fire models, Fire studies, Computer codes.

With a variety of objectives in mind, many different compartment fire model computer codes have been developed within the fire safety/research community. Yet, no one of these can be described as being a 'benchmark' model in the sense that it is reliable enough to be accepted as a standard of reference for the performance of design-oriented fire models. It is the major objective of the Compartment Fire Modeling Research (CFMR) Group in the Fire Safety Technology Division of the Center for Fire Research (CFR) to develop such a Benchmark Compartment Fire Model (BCFM) computer code. This paper describes the characteristics of this BCFM, and outlines the program which will lead to its development.

501,653
PB86-166659 PC A03/MF A01
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.
Forced Smolder Propagation and the Transition to Flaming in Cellulosic Insulation.
Final rept.,
T. J. Ohlemiller. Oct 85, 50p NBSIR-85/3212
Sponsored by Department of Energy, Washington, DC.

Keywords: *Insulation, *Combustion, Cellulose, Fire resistant coatings, Flame propagation, Flammability testing, Smoldering.

It is well known that a smoldering fuel responds to an increased oxygen supply by becoming faster and hotter until, eventually, flames erupt. This sequence is examined quantitatively for thick horizontal layers of a permeable fuel, i.e., cellulosic insulation. Two configurations are possible, forward and reverse smolder; both are investigated experimentally. The influence of combustion retardants is also investigated; these include boric acid, a smolder retardant; and borax, a flaming retardant. Both prevent the transition to flaming in the absence of adjacent flammable material but are less effective in its presence. The overall response of these various fuel mixtures and configurations suggests that both kinetics and oxygen supply rate (not the latter alone) play substantial roles in dictating smolder response to an air flow.

501,654
PB86-166667 PC A06/MF A01
National Bureau of Standards, Gaithersburg, MD. Ceramics Div.
Survey of Alternate Stored Chemical Energy Reactions.
Annual rept. 25 May 84-25 May 85,
L. P. Cook, and E. R. Plante. Dec 85, 107p NBSIR-85/3282
Contracts N00014-83-F-0117, N00014-84-F-0204
Sponsored by Office of Naval Research, Arlington, VA.

Keywords: *Liquid metals, *Combustion, Reaction kinetics, Enthalpy, Oxidation, Lithium, Aluminum, Boron, Beryllium, Magnesium, Nitrogen fluorides.

A survey of eight alternative liquid metal stored chemical energy reactions has been made for purposes of

comparison with the lithium-aluminum/water, lithium/sulfur hexafluoride, and other reaction schemes. The objective of the study was to survey the potential of these eight reactions as alternate stored chemical energy systems and to develop priorities for future study. Experimental data on the products of reaction and kinetics of reaction are presented for: (Li/H₂O; H₂/O₂), (Li/H₂O; NaO₂/H₂O; H₂/O₂), (MgAl/H₂O; H₂/O₂), and (LiAl/ClO₃F). These data have been collected using thermogravimetry and Knudsen effusion mass spectrometry, with x-ray diffraction analysis of experimental products. Among other results, the data show that the aluminum component of the fuels is relatively inert to oxidation up to 650 degrees C. Above this temperature, materials limitations have hampered the collection of experimental data. Thermodynamic analysis has been used to extend the data on each of the eight reaction schemes, and to predict the chemical reaction which best represents the complete oxidation of each fuel by the indicated oxidant at 1100 K. Enthalpies have been calculated for each fuel/oxidant combination. Safety considerations are also discussed for each.

501,655
PB86-170719 PC A02/MF A01
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.
Preliminary Analysis of Oil-Slick Combustion.
Final rept.,
I. S. Wichman. Nov 85, 20p NBSIR-85/3266
Sponsored by Minerals Management Service, Reston, VA.

Keywords: *Combustion, Ignition, Oil spills, Burning rate, *Oil slicks.

The preliminary study of oil-slick combustion contains a literature review, a formulation of a physical model of oil-slick burning, and some suggested experiments. The theoretical model is divided into three stages: (1) an ignition and acceleratory-growth stage; (2) a slow-down regime, in which finite slick thickness effects become important; and (3) an extinction cycle. The proposed experiments emphasize the use of the Fire Research Laboratory, located on the NBS grounds.

21D. Fuels

501,656
PB85-189421 Not available NTIS
National Bureau of Standards (NML), Gaithersburg, MD. Inorganic Analytical Research Div.
Determination of Ultratrace Levels of Lead in Reference Fuels by Graphite Furnace Atomic Absorption.
Final rept.,
M. S. Epstein. 1983, 2p
Pub. in At. Spectrosc. 4, n2 p62-63 1983.

Keywords: *Lead(Metal), *Trace elements, *Gasoline, *Chemical analysis, Standards, Exhaust emissions, Air pollution, Reprints, *Graphite furnace atomic spectroscopy, *Air pollution detection, Standard reference materials.

A modification of ASTM Standard Test Method D-1368-64 is used to determine levels of lead in isooctane and heptane less than a part-per-billion. The modification greatly simplifies the Test Method and reduces blank levels by almost two orders of magnitude. The accuracy of the method is confirmed by the determination of lead in NBS SRM 1636a (Lead in Reference Fuel).

501,657
PB85-206043 PC A08/MF A01
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Applied Mathematics.
MARKET: A Model for Analyzing the Production, Transmission, and Distribution of Natural Gas.
Technical note (Final),
C. Witzgall, and P. B. Saunders. Apr 85, 168p NBS/TN-1209
Also available from Supt. of Docs as SN003-003-02644-1. Sponsored by Department of Energy, Washington, DC.

Keywords: *Natural gas, *Gas industry, Gas production, Marketing, Gas distribution, Policies, Prices,

Supply(Economics), Demand(Economics), Regulations, Reserves, Mathematical models.

This report describes the MARKET submodel, one of three that combine to form the Gas Analysis Modeling System (GAMS). GAMS was developed for use by the Energy Information Administration of the U.S. Department of Energy. It provides a tool for analyzing the regional effects on the domestic natural gas market of various policies for regulating the price of natural gas at the wellhead. MARKET is concerned with the production of gas reserves and the transmission and distribution of gas to consumers. It solves a network equilibration problem to arrive at estimates of production quantities and prices.

501,658
PB85-207223 Not available NTIS

National Bureau of Standards (NML), Gaithersburg, MD. Organic Analytical Research Div.

Application of Perdeuterated Polycyclic Aromatic Hydrocarbons (PAH) as Internal Standards for the Liquid Chromatographic Determination of PAH in a Petroleum Crude Oil and Other Complex Mixtures.

Final rept.,
W. F. Kline, S. A. Wise, and W. E. May. 1985, 15p
Sponsored by Department of Energy, Washington, DC. Office of Health and Environmental Research.
Pub. in Jnl. of Liquid Chromatography 8, n2 p223-237 1985.

Keywords: *Aromatic polycyclic hydrocarbons, *Chromatographical analysis, *Standards, Chemical analysis, Petroleum products, Crude oil, Reprints, *Liquid chromatography, *Standard reference materials, Air pollution detection.

A sequential liquid chromatographic (LC) procedure for the determination of polycyclic aromatic hydrocarbons (PAH) in a petroleum crude oil and other complex mixtures is described. The procedure includes normal-phase LC on an anisilane column to isolate fractions containing isomeric PAH and reversed-phase LC on a polymeric C18 column to separate the individual PAH isomers. Appropriate perdeuterated PAH are added to the sample so that each isomeric fraction will contain one internal standard. The perdeuterated PAH are excellent internal standards for this sequential LC procedure. Perdeuterated PAH have normal-phase and reversed-phase LC retention characteristics similar to those of the parent PAH. In the normal-phase LC separation, the perdeuterated PAH elute in the same fraction as the parent PAH. In the reversed-phase LC separation, the perdeuterated PAH elute first and are generally resolved from the parent PAH. The optimized spectrofluorometric detection of each PAH analyte is accomplished by programming appropriate sets of excitation and emission wavelengths to correspond with the elution time of each analyte on the polymeric C18 column. The analytical results obtained from this procedure for the analysis of a shale oil sample (Standard Reference Material (SRM) 1580) and a petroleum crude oil (SRM 1582) are compared to values obtained by gas chromatography-mass spectrometry.

501,659
PB85-230860 Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

Speciation of Inorganic Arsenic and Organoarsenic Compounds in Fossil Fuel Precursors and Products.

Final rept.,
F. E. Brinckman, C. S. Weiss, and R. H. Fish. 1983, 19p

Sponsored by American Chemical Society, Washington, DC.
Pub. in Proceedings of the American Chemical Society Meeting Chemical Congress of the North American Continent, Las Vegas, Nevada, August 24, 1980, Chapter 13 in Chemical and Geochemical Aspects of Fossil Energy Extraction, p197-214 1983.

Keywords: *Arsenic inorganic compounds, *Arsenic organic compounds, *Fossil fuels, *Trace elements, Metal containing organic compounds, Chemical analysis, Atomic spectroscopy, Absorption spectra, Shale oil, Oil shale, Chemical reactions, Stability, Catalysts, *Chemical reaction mechanisms.

The molecular forms of trace metal(loid)s in fossil deposits are complex, probably consisting of varying proportions of inorganic, metallo-organic, and true organometallic chemical species residing in unspecified sites within the carbonaceous matrix. Modern industrial processing of fossil materials requires a refined understanding of the original form of the selected ele-

ment, its relationship to other matrix elements, and the pathways by which processing can alter the elements original form. From the standpoint of its environmental impact or its ability to poison catalysts used to upgrade crude oils, arsenic is a key element for which an urgent need exists to determine its chemical form(s) and transformations during fossil fuel processing. The underlying analytical requirements for the speciation of trace elements in fossil materials will be discussed along with a review of the present status of trace element speciation in these materials. Recent work performed in our laboratories on the speciation of arsenic compounds in shale oil, oil shale retort waters and oil shale kerogen is presented in this context.

501,660
PB86-102258 PC A06/MF A01

National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.

Development of a Model for the Heat Release Rate of Wood - A Status Report.

W. J. Parker. Jul 85, 107p NBSIR-85/3163
Contract EMW-E-1239

Keywords: *Wood, *Heats of combustion, *Mathematical models, Pyrolysis, Moisture contents, Exposure, Thermal conductivity, Fuels.

The report describes the status of the development of a method for predicting the heat release rate of wood for different thicknesses, moisture contents, and exposure conditions. A computer model has been set up on a microcomputer. Experimental techniques have been devised to obtain the input data required by the model. These include (1) the thermal conductivity as a function of temperature and percent loss, (2) the kinetic constants needed to describe the mass loss rate, (3) the heat of combustion of the volatile pyrolysis products, and (4) the contraction factors due to charring. Sufficient data on these parameters were taken to exercise the model. Heat release rates and effective heats of combustion were measured as a function of external radiant flux on 12.5 mm thick dry vertical specimens of Douglas fir particle board. The calculated and measured peak heat release rate curves are similar in shape and amplitude but differ significantly in time scale. This may be due to the lack of thermal conductivity data on the char in the high temperature range. There is very good agreement between the calculated and measured effective heats of combustion. The initial results with the model are promising.

501,661
PB86-102985 Not available NTIS

National Bureau of Standards (NEL), Boulder, CO. Chemical Engineering Science Div.

Thermal Conductivity of Coal-Derived Liquids and Petroleum Fractions.

Final rept.,
M. E. Baltatu, J. F. Ely, H. J. M. Hanley, M. S. Graboski, and R. A. Perkins. 1985, 8p

Sponsored by Gas Research Inst., Chicago, IL., and Department of Energy, Washington, DC. Office of Basic Energy Sciences.
Pub. in Industrial and Engineering Chemistry Process Design and Development 24, n2 p325-332 1985.

Keywords: *Petroleum products, *Thermal conductivity, *Coal liquids, Specific heat, Experimental data, Ideal gas, Comparison, Reprints, *Pseudopotential theory.

Thermal conductivity coefficients of coal-derived liquids and petroleum fractions are calculated by an extended corresponding states, conformal solution technique. The method requires as input pseudocritical parameters, molecular weight and acentric factor, and a pseudo-ideal gas heat capacity for each pseudocomponent or fraction. These quantities are estimated here from the mean average boiling point and specific gravity of the fractions using the techniques proposed by Riazi-Daubert, Kesler-Lee, and Winn: the relationship between the estimated conductivity and the choice of the method is noted. Predicted thermal conductivities are compared with data for three coal liquid samples measured at the Colorado School of Mines and with literature data. Agreement between prediction and experiment is generally within 10%, depending on the method used to calculate the input parameters. Some literature petroleum fractions data are also compared with the model. Again, agreement is within 10%.

501,662
PB86-110095 Not available NTIS

National Bureau of Standards, Boulder, CO. Fracture and Deformation Div.

Internal Friction and Dynamic Young Modulus of a Bituminous Coal.

Final rept.,
H. M. Ledbetter, M. W. Austin, and J. E. Callanan. 1985, 7p
Pub. in Proceedings of the American Chemical Society Fuel Division Symposium on Physical Methods for Fossil Fuels, Miami Beach, FL., April 28, 1985, American Chemical Society, Division of Fuel Chemistry 30, n1 p127-133 1985.

Keywords: *Bituminous coal, *Internal friction, *Modulus of elasticity, Physical properties, Polymers, Specific heat, Thermal expansion, Debye temperature.

Internal friction provides a well-known probe of defects in solids. The companion property--elastic modulus--provides valuable material characterization. This modulus relates in turn to a wide variety of other solid-state physical properties: specific heat, thermal expansivity, Debye temperature. Here the authors report preliminary measurements of these two physical properties between 295 and 76 K. Specimens consisted of square-cross-section rods approximately 5 mm by 30 mm. Apparatus consisted of a Marx oscillator at frequencies near 50 kHz. They found two internal-friction peaks, one centered near 220 K and one below 76 K. The preliminary results support the view that coal exhibits strong polymeric character.

501,663
PB86-119245 Not available NTIS

National Bureau of Standards, Gaithersburg, MD.

Evaluation of Data on Higher Heating Values Determined during ASTM (American Society for Testing and Materials) Round Robin Testing of RDF-3 (Refuse-Derived-Fuel).

Final rept.,
E. S. Domalski, and S. Abramowitz. Nov 80, 15p

Sponsored by Department of Energy, Washington, DC. Energy from Municipal Waste Div.
Pub. in Proceedings of Mineral Waste Utilization Symposium, Mineral and Mineral Process Waste - Urban Solid Waste - Industrial Waste Recovery - Scrap Metal Recovery, Chicago, IL., October 20-21, 1980, p69-83.

Keywords: *Standards, *Calorific value, Substitutes, Fuels, Chemical properties, Coal, Comparison, Tables(Data), Marketing, Statistical analysis, *Refuse derived fuels, *Round Robin tests, *Waste utilization, *Resource recovery facilities.

The potential application of RDF-3 as an alternative or supplemental fuel is dependent upon its acceptance as an article of commerce. ASTM Committee E-38 on Resource Recovery and its Subcommittee on Energy E-38.01 has been actively engaged in the development of consensus standards for this purpose since April 1974. Standard procedures for the characterization of RDF-3 are being developed. These procedures are based on those ASTM methods used in coal analysis. The procedures developed will insure a meaningful purchase - sales relationship between the buyer and seller. A variety of chemical and physical test procedures were studied by as many as 12 laboratories. Currently 20 editorial draft standards have been prepared and are being studied by the committee membership. The National Bureau of Standards in cooperation with ASTM subcommittee E38.01 has undertaken a technical review of a selected group of chemical properties of RDF-3. The property of principal interest is the higher heating value. In order to properly characterize this property, critical evaluation of methods to determine total moisture, residual moisture, and ash is also necessary. Intralab and interlab variations in these properties are discussed. A comparison of these results with those on round robin data for coal are also made. The results of this study identify the levels of precision for intralab and interlab agreement.

501,664
PB86-162112 Not available NTIS

National Bureau of Standards (NEL), Boulder, CO. Chemical Engineering Science Div.

LNG (Liquefied Natural Gas) Property Data and Metrology Technology.

Final rept.,
D. Mann, and J. A. Brennan. 1985, 10p
Sponsored by Groupe Internationale des Importateurs de Gas Natural Liquefie, and Southern California Gas Co., Los Angeles.

Field 21—PROPULSION AND FUELS

Group 21D—Fuels

Pub. in Proceedings of the World Gas Conference (16th), Munich, West Germany, June 24-27, 1985, p1-10.

Keywords: *Liquefied natural gas, Chemical properties, Reviews, Physical properties, Technology, Measurement instrumentation, Tables(Data).

Results of National Bureau of Standards (NBS) research programs concerning Liquefied Natural Gas (LNG) are presented and reviewed. In addition to previously reported information on LNG materials and fluids property data in graphic format, these more recent programs provide information on combustion enthalpies of the LNG components and mixtures for molecular weights of methane through the hexanes, real gas mixture densities, both measured and calculated and other thermophysical properties correlations, tabulations, and equations of state. The metrology of custody transfer is presented in context of previously completed NBS research programs dealing with LNG. These include LNG sampling and analysis, LNG density measurement both direct and calculated, liquid level instrumentation, ship and shore tank strapping and liquid flowmetering. Each of these measurement processes are examined for accuracy and precision. Propagation of error is presented with sample calculations and assessed for the various custody transfer situations such as ship tank unloading, pipeline flowmetering, shore tank storage and vaporization and gas flow measurements.

22. SPACE TECHNOLOGY

22B. Spacecraft

501,665
PB85-195899 Not available NTIS
National Bureau of Standards (NEL), Boulder, CO.
Vortex Shedding Flowmeters for Liquids at High Flow Velocities.
Final rept.,
J. D. Siegwarth. 1984, 8p
Sponsored by National Aeronautics and Space Administration, Huntsville, AL. Marshall Space Flight Center.

Pub. in Proceedings of MSFC Advanced High Pressure O₂H₂ Technology Conference 1984, Marshall Space Flight Center, Huntsville, AL., June 27-29, 1984 p33-339.

Keywords: *Flowmeters, Liquids, Flow measurement, Velocity, Liquid oxygen, Tests, Vanes, *Vortex shedding, *Space shuttle main engine.

A number of vortex shedding flowmeter designs for flow measurements in liquid oxygen ducts on the space shuttle main engines have been tested in a high head water flow test facility.

501,666
PB85-224400 PC A04/MF A01
National Bureau of Standards (NEL), Gaithersburg, MD. Center for Fire Research.
Slide-Rule Estimates of Fire Growth,
J. R. Lawson, and J. G. Quintiere. Jun 85, 57p
NBSIR-85/3196
Sponsored by David W. Taylor Naval Ship Research and Development Center, Bethesda, MD.

Keywords: *Flame propagation, Temperature, Carbon monoxide, Calculators, Estimates, Predictions, Computation, Fires, Smoke, *Fire growth, Fire models, Compartment fires.

A series of prediction methods have been assembled to provide an analytical basis for estimating fire growth in compartments. Solutions for each prediction method can be made using programmable scientific calculators. Prediction methods are presented for: fire size and growth rates, mass loss rates, radiant heat flux, flame height, radial flame impingement, heat flux to a ceiling, smoke filling of a room, carbon monoxide hazard with smoldering fires, temperature rise in a compartment, ventilation flow rate, flashover occurrence, corridor smoke transfer and filling, smoke concentration, visibility, flame spread rates, and fire burn time. These predictive methods are useful for estimating many of the critical elements related to fire behavior and help provide a better understanding of this complex phenomenon. This report appears in Appendix B in Fire Growth in Combat Ships by J.G. Quintiere, H.R. Baum and J.R. Lawson, NBSIR 85-3159.

501,667
PB86-100682 PC A06/MF A01
National Bureau of Standards (NEL), Boulder, CO. Chemical Engineering Science Div.
Cryogenic Propellant Scavenging. Final Report August 1982 - March 1985,
B. Louie, N. J. Kemp, and D. E. Daney. Apr 85, 123p
NBSIR-85/3023
Contract NASA-T-6077-J
Sponsored by National Aeronautics and Space Administration, Houston, TX. Lyndon B. Johnson Space Center.

Keywords: *Cryogenic rocket propellants, *Scavenging, Liquid propellants, Mathematical models, Pumps, Fuel tanks, Propellant transfer, Equations, Reduced gravity, Leakage, Temperature, Transferring, Thermodynamics, Computer programs, Cryogenic fluids, Space shuttles, Computer applications.

The report is a detailed description of a computer model that has been developed for assessing the feasibility of low g cryogen propellant scavenging from the Space Shuttle External Tank (ET). Either pump-assisted or pressure-induced propellant transfer may be selected. The program will accept a wide range of input variables, including the fuel to be transferred (LOX or LH₂), heat leaks, tank temperatures, and piping and equipment specifications. The model has been parametrically analyzed to determine initial design specification for the system.

22C. Spacecraft Trajectories and Reentry

501,668
PB86-119351 Not available NTIS
National Bureau of Standards, Gaithersburg, MD.
Elimination of the Parallax in Satellite Theory.
Final rept.,
A. Deprit. 1981, 43p
Pub. in Celestial Mechanics 24, p111-153 Jun 81.

Keywords: *Orbits, *Parallax, Perturbation theory, Removal, Elimination, Reprints, *Satellite orbits, Lie transformation.

When the perturbation affecting a Keplerian motion is proportional to $(r \supset -n)(n = \text{or } > 3)$, a canonical transformation of Lie type will convert the system into one in which the perturbation is proportional to $(r \supset -2)$. Because it removes parallax factors, the transformation is called the elimination of the parallax. In the main problem for the theory of artificial satellites, the elimination of the parallax has been conducted by computer to order 4. The first order in the reduced system may now be integrated in closed form, thereby revealing the fundamental property of the first-order intermediary orbits in line with Newton's Proposition XLIV. Extension beyond order 1 leads to identify a new class of intermediaries for the main problem in nodal coordinates, namely the radial intermediaries. The technique of smoothing a perturbation prior to normalizing the perturbed Keplerian system, of which the elimination of the parallax is an instance, is applied to derive the intermediaries in nodal coordinates proposed by Sterne, Garfinkel, Cid-Palacios and Aksnes, and to find the canonical diffeomorphisms which relate them to one another and to the radial intermediaries.

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PB86-136629

500,049

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Title
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PB86-165859 Use of Kalman Filtering and Correlation Techniques in Analytical Calibration Procedures, PB86-165867 (Order as PB86-165776, PC A08/MF A01)	500,602	(Order as PB86-165776, PC A08/MF A01)	
PB86-165867 Use of Kalman Filtering and Correlation Techniques in Analytical Calibration Procedures, PB86-165867 (Order as PB86-165776, PC A08/MF A01)	501,332		
PB86-165875 Intelligent Instrumentation, PB86-165875 (Order as PB86-165776, PC A08/MF A01)	501,333		
PB86-165883 Regression Analysis of Collinear Data, PB86-165883 (Order as PB86-165776, PC A08/MF A01)	500,967		
PB86-165891 Optimization, PB86-165891 (Order as PB86-165776, PC A08/MF A01)	501,334		
PB86-165909 Strategies for the Reduction and Interpretation of Multicomponent Spectral Data, PB86-165909 (Order as PB86-165776, PC A08/MF A01)	500,603		
PB86-165917 Some New Ideas in the Analysis of Screening Designs, PB86-165917 (Order as PB86-165776, PC A08/MF A01)	500,968		
PB86-165925 Polymers and Random Walks - Renormalization Group Description and Comparison with Experiment, PB86-165925 (Order as PB86-165776, PC A08/MF A01)	500,604		
PB86-165933 Fourier Representations of Pdf's Arising in Crystallography, PB86-165933 (Order as PB86-165776, PC A08/MF A01)	501,419		
PB86-165941 Aggregated Markov Processes and Channel Gating Kinetics, PB86-165941 (Order as PB86-165776, PC A08/MF A01)	500,605		
PB86-165958 Automated Pattern Recognition: Self-Generating Expert Systems for the Future, PB86-165958 (Order as PB86-165776, PC A08/MF A01)	500,606		
PB86-165966 Regression Analysis of Compartmental Models, PB86-165966 (Order as PB86-165776, PC A08/MF A01)	500,969		
PB86-165974 Measurement and Control of Information Content in Electrochemical Experiments, PB86-165974	500,607		
PB86-165982 Pattern Recognition Studies of Complex Chromatographic Data Sets, PB86-165982 (Order as PB86-165776, PC A08/MF A01)	500,608		
PB86-166196 Naval Fire Fighting Trainers: Effect of Ventilation on Fire Environment (Model Calculations for 19F3 FFT), PB86-166196 (Order as PB86-165776, PC A08/MF A01)	501,118	PC A03/MF A01	
PB86-166592 Program for the Development of a Benchmark Compartment Fire Model Computer Code, PB86-166592 (Order as PB86-165776, PC A08/MF A01)	501,652	PC A03/MF A01	
PB86-166600 Estimating Interroom Contaminant Movements, PB86-166600 (Order as PB86-165776, PC A08/MF A01)	501,022	PC A03/MF A01	
PB86-166626 Indoor Air Quality Modeling, Phase 1 Report. Framework for Development of General Models, PB86-166626 (Order as PB86-165776, PC A08/MF A01)	501,023	PC A04/MF A01	
PB86-166634 CSFIT: A FORTRAN Program for Charge-Sheet Model Fitting of MOSFET Data, PB86-166634 (Order as PB86-165776, PC A08/MF A01)	500,657	PC A03/MF A01	
PB86-166642 Fire Behavior of Upholstered Furniture, PB86-166642 (Order as PB86-165776, PC A08/MF A01)	500,862	PC A06/MF A01	
PB86-166659 Forced Smolder Propagation and the Transition to Flaming in Cellulosic Insulation, PB86-166659 (Order as PB86-165776, PC A08/MF A01)	501,653	PC A03/MF A01	
PB86-166667 Survey of Alternate Stored Chemical Energy Reactions, PB86-166667 (Order as PB86-165776, PC A08/MF A01)	501,654	PC A06/MF A01	
PB86-166725 Finline Diode Six-Port: Fundamentals and Design Information, PB86-166725 (Order as PB86-165776, PC A08/MF A01)	501,335	PC A03/MF A01	
PB86-166774 NBS*LATTICE - A Program to Analyze Lattice Relationships. Version of Summer, 1985. PB86-166774 (Order as PB86-165776, PC A08/MF A01)	501,420	PC A05/MF A01	
PB86-166782 Journal of Research of the National Bureau of Standards, Volume 90, Number 5, September-October 1985. PB86-166782 (Order as PB86-165776, PC A08/MF A01)	501,336	PC A04/MF A01	
PB86-166790 Note on Weighings Carried Out on the NBS-2 Balance, PB86-166790 (Order as PB86-166782, PC A04/MF A01)	501,337		
PB86-166808 Thermodynamics of Solution of SO ₂ (g) in Water and of Aqueous Sulfur Dioxide Solutions, PB86-166808	500,609		
PB86-166816 SRM 1970: Succinonitrile Triple-Point Standard - A Temperature Reference Standard Near 58.08C, PB86-166816 (Order as PB86-166782, PC A04/MF A01)	501,338		
PB86-166824 Performance Assessment of Automatic Speech Recognizers, PB86-166824 (Order as PB86-166782, PC A04/MF A01)	501,350		
PB86-166832 Chemical Kinetics - Theory and Experiment, PB86-166832 (Order as PB86-166782, PC A04/MF A01)	500,610		
PB86-166998 Roof Management Programs, PB86-166998 (Order as PB86-166782, PC A04/MF A01)	501,152	PC A04/MF A01	
PB86-167327 Possible Estimation Methodologies for Electromagnetic Field distributions in Complex Environments, PB86-167327 (Order as PB86-166782, PC A04/MF A01)	501,430	PC A04/MF A01	
PB86-167863 NBS (National Bureau of Standards) Reactor: Summary of Activities July 1984 through June 1985, PB86-167863 (Order as PB86-166782, PC A04/MF A01)	501,612	PC A09/MF A01	
PB86-169083 Site Attenuation, PB86-169083 (Order as PB86-166782, PC A04/MF A01)	500,789	PC A04/MF A01	
PB86-169109 Construction Materials for Coal Conversion: Performance and Properties Data. Supplement 2. PB86-169109 (Order as PB86-166782, PC A04/MF A01)	501,040	PC A99/MF E04	
PB86-170719 Preliminary Analysis of Oil-Slick Combustion, PB86-170719 (Order as PB86-166782, PC A04/MF A01)	501,655	PC A02/MF A01	
PB86-174505 Piezoelectric Polymer Heat Exchanger. PATENT-4 501 319 (Order as PB86-166782, PC A04/MF A01)	500,975	Not available NTIS	
PB86-174513 Radiochromic Leuko Dye Real Time Dosimeter, One Way Optical Waveguide. PATENT-4 489 240 (Order as PB86-166782, PC A04/MF A01)	500,115	Not available NTIS	
PB86-174521 Bond Testing Apparatus. PATENT-4 491 014 (Order as PB86-166782, PC A04/MF A01)	501,154	Not available NTIS	
PB86-174539 Fluid Safety Valve. PATENT-4 494 563 (Order as PB86-166782, PC A04/MF A01)	501,081	Not available NTIS	
VPI-E-85-5 Thermal Performance Testing and Mathematically Modeling of Integral Collector Storage Solar Hot Water Systems. PB85-186906	501,119	PC A11/MF A01	

APPENDIX A

List of Depository Libraries in the United States

ALABAMA

Alexander City

Alexander City State Junior College Thomas S. Russell Library (1967)*

Auburn

Auburn University Ralph Brown Draughon Library (1907)

Birmingham

Birmingham Public Library (1895)
Birmingham-Southern College Library (1932)
Jefferson State Junior College James B. Allen Library (1970)
Miles College C. A. Kirkendoll Learning Resource Center (1980)
Samford University 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)
Auburn 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)

* Year designated.

Troy

Troy State University Library (1963)

Tuskegee Institute

Tuskegee Institute Hollis Burke Frissell Library (1907)

University

University of Alabama Library (1860) REGIONAL
University of Alabama School of Law Library (1967)

ALASKA

Anchorage

Anchorage Law Library (1973)
Anchorage Municipal Libraries Z. J. Loussac Public Library (1978)
University of Alaska at Anchorage Library (1961)
U.S. Department of Interior Alaska Resources Library (1981)
U.S. District Court Library (1983)

Fairbanks

University of Alaska Elmer E. Rasmuson Library (1922)

Juneau

Alaska State Library (1900)
University of Alaska-Juneau Library (1981)

Ketchikan

Ketchikan Community College Library (1970)

AMERICAN SAMOA

Pago Pago

Community College of American Samoa Library (1985)

ARIZONA

Coolidge

Central Arizona College (1973)

Flagstaff

Northern Arizona University Library (1937)

Holbrook

Northland Pioneer College (1985)

Mesa

Mesa Public Library (1983)

Phoenix

Department of Library Archives, and Public Records (unknown)
REGIONAL

Grand Canyon College Fleming Library (1978)

Phoenix Public Library (1917)

U.S. Court of Appeals (1984)

Prescott

Yavapai College Library (1976)

Tempe

Arizona State University College of Law Library (1977)

Arizona State University Library (1944)

Tucson

Tucson Public Library (1970)

University of Arizona Library (1907) REGIONAL

Yuma

Yuma City-County Library (1963)

ARKANSAS

Arkadelphia

Ouachita Baptist University Riley Library (1963)

Batesville

Arkansas College Library (1963)

Clarksville

College 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 (1978)

Little Rock

Arkansas State Library (1978) REGIONAL

Arkansas Supreme Court Library (1962)

Little Rock Public Library (1953)

University of Arkansas at Little Rock Library (1973)

University of Arkansas at Little Rock, School of Law Library (1979)

Magnolia

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 Tech University Tomlinson Library (1925)

Searcy

Harding University Beaumont Memorial Library (1963)

State University

Arkansas State University Dean B. Ellis Library (1913)

Walnut Ridge

Southern Baptist College Felix Goodson Library (1967)

CALIFORNIA

Anaheim

Anaheim Public Library (1963)

Arcadia

Arcadia Public Library (1975)

Arcata

Humboldt State University Library (1963)

Bakersfield

California State College Bakersfield Library (1974)

Kern County, Beale Memorial Library (1943)

Berkeley

University of California General Library (1907)

University of California Law Library (1963)

Carson

California State University Dominguez Hills Educational Resources Center (1973)

Carson Regional Library (1973)

Chico

California State University Merriam Library (1962)

Claremont

Claremont Colleges' Libraries Honnold Library (1913)

Compton

Compton Public Library (1972)

Culver City

Culver City 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)
Fresno County Free Library (1920)

Fullerton

California State University at Fullerton Library (1963)
Western State University College of Law Library (1984)

Garden Grove

Garden Grove Regional Library (1963)

Gardena

Gardena Public Library (1966)

Hayward

California State University at Hayward Library (1963)

Huntington Park

Huntington Park Library (1970)

Inglewood

Inglewood Public Library (1963)

Irvine

University of California at Irvine General 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 at Los Angeles John F. Kennedy Memorial 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 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 9th Circuit Library (1981)
Whittier College School of Law Library (1978)

Malibu

Pepperdine University Payson Library (1963)

Menlo Park

Department of Interior 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 Hill

Contra Costa County Library (1964)

Redding

Shasta County Library (1956)

Redlands

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 at Sacramento Library (1963)
Sacramento County Law Library (1963)
Sacramento Public Library (1880)
University of the Pacific McGeorge School of Law Library (1978)

San Bernardino

San Bernardino County Law Library (1984)
San Bernardino County Library (1964)

San Diego

San Diego County Law Library (1973)
San Diego County Library (1966)
San Diego Public Library (1895)
San Diego State University Library (1962)
University of San Diego Kratter Law Library (1967)

San Francisco

Golden Gate University School of Law Library (1979)
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 Library (1962)

San Leandro

San Leandro Community Library Center (1961)

San Luis Obispo

California Polytechnic State University Robert E. Kennedy Library (1969)

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

University of Santa Clara 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 College Library (1964)

Torrance

Torrance Public Library (1969)

Turlock

California State College 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)

Whittier

Whittier College Wardman Library (1963)

CANAL ZONE

Balboa Heights

Panama Canal Commission (1963)

COLORADO

Alamosa

Adams State College Library (1963)

Aurora

Aurora Public Library (1984)

Boulder

University of Colorado at Boulder Norlin Library (1879) REGIONAL

Colorado Springs

Colorado College Tutt Library (1880)
University of Colorado at Colorado Springs Library (1974)
U.S. Air Force Academy Academy Library (1956)

Denver

Auraria Library (1978)
Colorado State Library (unknown)
Colorado Supreme Court Library (1978)
Denver Public Library (1884) REGIONAL
Department of the Interior Bureau of Reclamation Library (1962)
Regis College Dayton Memorial Library (1915)
U.S. Court of Appeals Tenth Circuit 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 College Lowell Heiny Library (1978)

Greeley

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)

Danielson

Quinebaug Valley Community College Audrey P. Beck Library (1975)

Enfield

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)

Mystic

Mystic Seaport Museum, Incorporated 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 (1977)
Silas Bronson Public Library (1869)

West Haven

University of New Haven Peterson Library (1971)

DELAWARE

Dover

Delaware State College William C. Jason Library (1962)
State Law Library in Kent County (unknown)

Georgetown

Delaware Technical and Community College Library (1968)
Sussex County Law Library (1976)

Newark

University of Delaware Library (1907)

Wilmington

Delaware Law School Library (1976)
New Castle County Law Library (1974)

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)
Antioch School of Law Library (1982)
Catholic University of America Robert J. White Law Library (1979)
Department of the Army Pentagon Library ANRAL (1969)
Department of Commerce Library (1955)
Department of Health and Human Services Library (1954)
Department of Housing and Urban Development Library (1969)
Department of the Interior Library 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 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, Office of Administration, Library & Information Service Division (1965)
Federal Deposit Insurance Corporation Library (1972)
Federal Election Commission Library (1975)
Federal Energy Regulatory Commission Library (1983)
Federal Labor Relations Authority Law Library (1982)
Federal Mine Safety & Health Review Commission Library (1979)
Federal Reserve System Board of Governors Research Library (1978)
Federal Reserve System Law Library (1976)
General Accounting Office Library (1974)
General Services Administration Library (1975)
Georgetown University Library (1969)
Georgetown University Law Center Fred O. Dennis Law 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. 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 (1970)
Veterans' Administration Central Office Library (1967)

FLORIDA

Boca Raton

Florida Atlantic University S. E. Wimberly Library (1963)

Clearwater

Clearwater Public Library (1972)

Coral Gables

University of Miami Library 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, Center for Study of Law/Law Library (1967)

Fort Pierce

Indian River Community College Library (1975)

Gainesville

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)

Lakeland

Lakeland Public Library (1928)

Leesburg

Lake-Sumter Community College Library (1963)

Melbourne

Florida Institute of Technology Library (1963)

Miami

Florida International University Library (1970)
Miami-Dade Public Library (1952)

North Miami

Florida International University North Miami 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 County Library System (1973)

Saint Petersburg

Saint Petersburg Public Library (1965)
Stetson University College of Law Charles A. Dana Library (1975)

Sarasota

Selby Public Library (1970)

Tallahassee

Florida Agricultural and Mechanical University Coleman Memorial Library (1936)
Florida State University College of Law Library (1978)
Florida State University Stroz 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 Mills Memorial 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 School of Law Library (1968)
Emory University Woodruff Library (1928)
Georgia Institute of Technology Price Gilbert Memorial Library (1963)
Georgia State 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)

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 Junior College Library Resource Center (1978)

Macon

Mercer University Stetson Memorial Library (1964)
Mercer University Walter F. George School of Law Library (1978)

Marietta

Kennesaw College Library (1968)

Milledgeville

Georgia College at Milledgeville Ina Dillard Russell Library (1950)

Mount Berry

Berry College Memorial Library (1970)

Savannah

Chatham-Effingham Liberty Regional Library (1857)

Statesboro

Georgia Southern College Liberty (1939)

Valdosta

Valdosta State College Library (1956)

GUAM

Agana

Nieves M. Flores Memorial Library (1962)

Mangilao

University of Guam Robert F. Kennedy Memorial Library (1978)

HAWAII

Hilo

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)

Laie

Brigham Young University Hawaii Campus, Joseph F. Smith Library (1964)

Lihue

Kauai Regional Library (1967)

Pearl City

Leeward Community College Library (1967)

Wailuku

Maul Public Library (1962)

IDAHO

Boise

Boise Public Library and Information Center (1929)
Boise State University Library (1966)
Idaho State Law Library (unknown)
Idaho State Library (1971)

Caldwell

College of Idaho Terteling Library (1930)

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 Oboier Library (1908)

Rexburg

Ricks College David O. McKay Learning Resources Center (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)

Cartersville

Shawnee Library System (1971)

Champaign

University of Illinois Law Library (1965)

Charleston

Eastern Illinois University Booth Library (1962)

Chicago

Chicago Public Library (1876)
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 Library (1961)
Northwestern University School of Law Library (1978)
University of Chicago Law Library (1964)
University of Chicago Library (1897)
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

Oakton Community College Library (1976)

Edwardsville

Southern Illinois University 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 College Benner Library and Learning Resource 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 Library (1972)

Peoria

Bradley University Cullom-Davis Library (1963)
Peoria Public Library (1883)

River Forest

Rosary College Library Rebecca Crown Library (1966)

Rockford

Rockford Public Library (1895)

Romeoville

Lewis University Library (1952)

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)

Bloomington

Indiana University Library (1881)
Indiana University Law Library (1978)

Crawfordsville

Wabash College Lilly Library (1906)

Evansville

Evansville and Vanderburgh County Public Library (1928)
Indiana State University at Evansville Evansville Campus Library (1969)

Fort Wayne

Allen County Public Library (1896)
Indiana University-Purdue University at Fort Wayne Helmke Library (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 Loew Alumni 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)

Muncie

Ball State University Alexander M. Bracken Library (1959)
Muncie Public Library (1906)

New Albany

Indiana University Southeastern Library (1965)

Notre Dame

University of Notre Dame Memorial 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 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 Library (1907)

Cedar Falls

University of Northern Iowa Library (1946)

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

Grinnel College Burling Library (1874)

Iowa City

University of Iowa College of Law 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)

Sioux City

Sioux City Public Library (1894)

KANSAS

Atchison

Benedictine College Library (1965)

Baldwin City

Baker University Collins Library (1908)

Colby

Colby Community College H.F. Davis Memorial Library (1968)

Emporia

Emporia State University William Allen White Library (1909)

Hays

Fort Hays State University Forsyth Library (1926)

Hutchinson

Hutchinson Public Library (1963)

Fort Scott

Fort Scott Community College Learning Resources Center Library (1979)

Lawrence

University of Kansas Law Library (1971)

University of Kansas Spencer Research Library (1869) REGIONAL

Manhattan

Kansas State University Farrell Library (1907)

Pittsburg

Pittsburg State University Leonard H. Axe Library (1952)

Salina

Kansas Wesleyan 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

Boyd County Public Library (1946)

Barbourville

Union College Abigail E. Weeks Memorial Library (1958)

Bowling Green

Western Kentucky University Helm-Cravens Library (1934)

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)

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 Memorial Library (1983)

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 Law School Library (1979)

Southern University Library (1952)

Eunice

Louisiana State University at Eunice LeDoux Library (1969)

Hammond

Southeastern Louisiana University Sims Memorial Library (1966)

Lafayette

University of Southwestern Louisiana Library (1938)

Lake Charles

McNeese State University Lether E. Frazar Memorial Library (1941)

Monroe

Northeast Louisiana University Sandel Library (1963)

Natchitoches

Northwestern State University of Louisiana Watson Memorial Library (1887)

New Orleans

Law Library of Louisiana (unknown)

Loyola University 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 (1942)

Tulane University Howard-Tilton Memorial Library (1884)

U.S. Court of Appeals Fifth 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)

Baltimore

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 Air

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 McKeldin Library (1925) REGIONAL

Cumberland

Allegheny Community College Library (1974)

Frostburg

Frostburg State College Library (1967)

Patuxent River

Patuxent River Central Library (1968)

Rockville

Montgomery County Department of Public Libraries (1951)

Salisbury

Salisbury State College Blackwell Library (1965)

Towson

Goucher College Julia Rogers Library (1966)

Towson State University Cook Library (1979)

Westminister

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 Pappas Law Library (1979)

Northeastern University Dodge 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 Libraries (1946)

Chicopee

College of Our Lady of the Elms, Alumnae Library (1969)

Lowell

University of Lowell Alumni-Lydon Library (1952)

Lynn

Lynn Public Library (1963)

Medford

Tufts University Wessel Library (1899)

Milton

Curry College, Levin Library (1972)

New Bedford

New Bedford Free Public Library (1858)

Newton

Boston College Thomas P. O'Neill Jr. Library (1963)

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 Law Library (1978)

Waltham

Brandeis University Library (1965)

Waltham Public Library (1982)

Wellesley

Wellesley College Library (1943)

Wenham

Gordon College Winn Library (1963)

Williamstown

William College Library (unknown)

Worcester

American Antiquarian Society Library (1814)

University of Massachusetts Medical Center Lamar Soutter Library (1972)

Worcester Public Library (1859)

MICHIGAN

Albion

Albion College Stockwell Memorial 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)

Bloomfield 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 G. Flint Purdy Library (1937)

Wayne State University Arthur Neef Law Library (1971)

Dowagiac

Southwestern Michigan College Matthews Library (1971)

East Lansing

Michigan State University 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 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

Schoolcraft College Library (1962)

Madison Heights

Madison Heights Public Library (1982)

Marquette

Northern Michigan University Olson Library (1963)

Monroe

Monroe County Library System (1974)

Mount Clemens

Macomb County Library (1968)

Mount Pleasant

Central Michigan University Library (1958)

Muskegon

Hackley Public Library (1894)

Olivet

Olivet College Library (1974)

Petoskey

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 College Kenneth Shouldice Library (1982)

Traverse City

Northwestern Michigan College Mark Osterlin Library (1964)

University Center

Delta College Learning Resources Center (1963)

Warren

Warren Public Library Arthur J. Miller Branch (1973)

Wayne

Wayne Oakland Library Federation (1957)

Ypsilanti

Eastern Michigan University Library (1965)

MICRONESIA

Community College of Micronesia Library (1982)

MINNESOTA

Bemidji

Bemidji 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 (1983)

Duluth

Duluth Public Library (1909)

University of Minnesota, Duluth Library (1984)

Eagan

Dakota County Eagan Library (1983)

Edina

Southdale-Hennepin Area Library (1971)

Mankato

Mankato State University Library (1962)

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 Resources 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 Library (1941)

Willmar

Pioneerland Library (1958)

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)

Hattiesburg

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 Library (1970)

Mississippi State

Mississippi State University Mitchell Memorial Library (1907)

Pascagoula

Jackson-George Regional Library (1985)

University

University of Mississippi J. D. Williams Library (1883) REGIONAL

University of Mississippi James O. Eastland Law Library (1967)

MISSOURI

Cape Girardeau

Southeast Missouri State University Kent Library (1916)

Columbia

University of Missouri at Columbia Library (1862)

University of Missouri-Columbia Law Library (1978)

Fayette

Central Methodist College George M. Smiley Library (1962)

Fulton

Westminster College Reeves Library (1875)

Hillsboro

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 Library (1966)

Kansas City

Kansas City Missouri Public Library (1881)

Rockhurst College Greenleaf 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

Lindenwood College Margaret Leggat Butler Library (1973)

Saint Joseph

Saint Joseph Public Library (1891)

Saint Louis

Marysville 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 Library (1963)

Warrensburg

Central Missouri State University Ward Edwards Library (1914)

MONTANA

Billings

Eastern Montana College Library (1958)

Bozeman

Montana State University Renne Library (1907)

Butte

Montana College of Mineral Science and Technology Library (1901)

Havre

Northern Montana College Vande Bogart Library (1980)

Helena

Carroll College Library (1974)

Montana State Library (1966)

State Law Library of Montana (1977)

Missoula

University of Montana Maurene & Mike Mansfield Library (1909)
REGIONAL

NEBRASKA

Blair

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)

Wayne

Wayne State College U.S. Conn Library (1970)

NEVADA

Carson City

Nevada State Library (unknown)

Nevada Supreme Court Library (1973)

Las Vegas

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)

Bloomfield

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 Learning Resource Center (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

New Brunswick Free Public Library (1908)

Rutgers University Alexander Library (1907)

Newark

Newark Public Library (1906) REGIONAL

Rutgers-The State University of New Jersey John Cotton Dana Library (1966)

Rutgers University Law School, Ackerson Law Library (1979)

Seton Hall University Law Library (1979)

Passaic

Passaic Public Library (1964)

Pemberton

Burlington County College Library (1979)

Phillipsburg

Phillipsburg Free Public Library (1976)

Plainfield

Plainfield Public Library (1971)

Pomona

Stockton State College Library (1972)

Princeton

Princeton University 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 McLaughlin Library (1947)

Teaneck

Fairleigh Dickinson University Teaneck/Hackensack Campus Weiner Library (1963)

Toms River

Ocean County College Learning Resources Center (1966)

Trenton

**New Jersey State Library (unknown)
Trenton Free Public Library (1902)**

Union

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)**

Silver 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 Library (1979)
New York State Library (unknown) REGIONAL
State University of New York at Albany University Library (1964)**

Auburn

Seymour Library (1972)

Bayside

CUNY Law School at Queens College CUNY Law Library (1983)

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)
Herbert H. 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 Raushensh Library (1910)

Brooklyn

Brooklyn College Library (1936)
Brooklyn Law School Library (1974)
Brooklyn Public Library (1908)
Brooklyn Public Library Business Library (1984)
Pratt Institute Library (1891)
State University of New York Downstate Medical Center 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

Corning Community College Arthur A. Houghton Jr. Library (1963)

Cortland

State University of New York College at Cortland Memorial Library (1964)

Delhi

State University Agricultural and Technical College Library (1970)

Douglaston

Cathedral College Library (1971)

East Islip

East Islip Public Library (1973)

Elmira

Elmira College Gannett Tripp Learning Center (1956)

Farmingdale

State University of New York at Farmingdale Greenley Library (1917)

Flushing

Queens College Paul Klapper 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 School of Law Library (1985)

Ithaca

Cornell University Library (1907)
Cornell Law Library (1978)
New York State College of Agriculture and Human Ecology 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)

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 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)
Medical Library Center of New York (1976)
New York Law Institute Library (1909)
New York Law School Library (1979)
New York Public Library (1907)
New York Public Library (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 Cordoza 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 Oneonta 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 Harriet Call Burnap Memorial Library (1938)

State University College at Potsdam Frederick W. Crumb Memorial Library (1964)

Poughkeepsie

Vassar College Library (1943)

Purchase

State University of New York, College of 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 Southampton Campus Library (1973)

Sparkill

St. Thomas Aquinas College Loughheed 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 Bird Library (1878)
Syracuse University College of Law H. Douglas Barclay Law Library (1978)

Troy

Troy Public Library (1869)

Uniondale

Nassau Library System (1965)

Utica

Utica Public Library (1885)
SUNY College of Technology Library (1977)

West Point

U.S. Military Academy Library (unknown)

White Plains

Pace University Law School 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)

Boiling Springs

Gardner-Webb College Dover Memorial Library (1974)

Boone

Appalachian State University Carol Grotnes Belk Library (1963)

Buies 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 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 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 Presbyterian College DeTamble Library (1969)

Lexington

Davidson County Public Library (1971)

Mount Olive

Mount Olive College Moye Library (1971)

Murfreesboro

Chowan College Whitaker Library (1963)

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)

Salisbury

Catawba College Library (1925)

Wilmington

University of North Carolina at Wilmington William M. Randall Library
(1965)

Wilson

Atlantic Christian College Hackney Library (1930)

Winston-Salem

Forsyth County Public Library (1954)

Wake Forest University Z. Smith Reynolds Library (1902)

NORTH DAKOTA

Bismarck

North Dakota State Library (1971)

North Dakota Supreme Court Law Library (unknown)

State Historical Society of North Dakota State Archives & Historical Research Library (1907)

Veteran's Memorial Public Library (1967)

Dickinson

Dickinson State College 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 College Memorial Library (1925)

Valley City

Valley City State College Library (1913)

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)

Alliance

Mount Union College Library (1888)

Ashland

Ashland College Library (1938)

Athens

Ohio University Alden Library (1886)

Batavia

University of Cincinnati at Batavia Clermont General and Technical College Library (1973)

Bluffton

Bluffton College, Musselman Library (1951)

Bowling Green

Bowling Green State University Jerome Library (1933)

Canton

Malone College Everett L. Cattell Library (1970)

Chardon

Geauga County Public Library (1971)

Cincinnati

Public Library of Cincinnati and Hamilton County (1884)

University of Cincinnati Central Library (1929)

University of Cincinnati College of Law (1978)

Cleveland

Case Western Reserve University Freiburger 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)

Ohio State University College of Law Library (1984)

Ohio State University Libraries (1907)

Ohio Supreme Court Law Library (1973)

Public Library of Columbus and Franklin County (1885)

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)

Elyria

Elyria Public Library (1966)

Findlay

Findlay College Shafer Library (1969)

Gambier

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)

Marietta

Marietta College Dawes Memorial Library (1884)

Marion

Marion Public Library (1979)

Middletown

Miami University-Middletown Gardner-Harvey Library (1970)

New Concord

Muskingum College Library (1966)

Oberlin

Oberlin College Library (1858)

Oxford

Miami University Libraries King Library (1909)

Portsmouth

Portsmouth Public Library (unknown)

Rio Grande

Rio Grande College and Community College Jeanette Albiez Davis Library (1966)

Springfield

Warder Public Library (1884)

Steubenville

University of Steubenville Starvaggi Memorial Library (1971)
Public Library of Steubenville and Jefferson County (1950)

Tiffin

Heidelberg College Beeghly Library (1964)

Toledo

Toledo-Lucas 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)

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

Bethany Nazarene College R. T. Williams Learning Resources Center (1971)

Durant

Southeastern Oklahoma State University Henry G. Bennett Memorial Library (1929)

Edmond

Central State University Library (1934)

Enid

Public Library of Enid and Garfield County (1908)

Langston

Langston University G. Lamar Harrison Library (1941)

Muskogee

Muskogee Public Library (1971)

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 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)

Corvallis

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)
Library Association of 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)

PENNSYLVANIA

Allentown

Muhlenberg College Haas Library (1939)

Altoona

Altoona Area Public Library (1969)

Bethel Park

Bethel Park Public Library (1980)

Bethlehem

Lehigh University Libraries Liderman Library (1876)

Blue Bell

Montgomery County Community College Learning Resources
Center (1975)

Bradford

University of Pittsburgh at Bradford Bradford Campus Library (1979)

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)

Coraopolis

Robert Morris College Library (1978)

Doylestown

Bucks County Free Library (1970)

East Stroudsburg

East Stroudsburg University Kemp Library (1966)

Erie

Erie County Library System (1897)

Greenville

Thiel College Langenheim Memorial Library (1963)

Harrisburg

State Library of Pennsylvania (unknown) REGIONAL

Haverford

Haverford College Magill Library (1897)

Hazleton

Hazleton Area Public Library (1964)

Indiana

Indiana University of Pennsylvania Rhodes R. Stabley Library (1962)

Johnstown

Cambria County Library System Glosser Memorial Library Building
(1965)

Lancaster

Franklin and Marshall College Shadek-Fackenthal Library (1895)

Lewisburg

Bucknell University Ellen Clarke Bertrand Library (1963)

Mansfield

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)

Newtown

Bucks County Community College Library (1968)

Norristown

Montgomery County Norristown Public Library (1969)

Philadelphia

Drexel University Library (1963)

Free Library of Philadelphia (1897)
 Saint Joseph's University Drexel Library (1974)
 Temple University Paley Library (1947)
 Temple University Law Library (1979)
 Thomas Jefferson University Scott Memorial Library (1978)
 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 (1895)
 Carnegie Library of Pittsburgh Allegheny Regional Branch (1924)
 Duquesne University Law Library (1978)
 La Roche College John J. Wright Library (1974)
 U.S. Department of Interior Bureau of Mines Library (1962)
 University of Pittsburgh Hillman Library (1910)
 University of Pittsburgh 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

Slippery Rock University 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)

Washington

Washington and Jefferson College U. Grant Miller Library (1884)

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)

Rio Piedras

University of Puerto Rico J. M. Lázaro Library (1928)

RHODE ISLAND

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

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 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 Larry A. Jackson Library (1967)

Orangeburg

South Carolina State College Miller F. Whittaker Library (1953)

Rock Hill

Winthrop College Dacus Library (1896)

Spartansburg

Spartansburg County Public Library (1967)

SOUTH DAKOTA

Aberdeen

Northern State College Beulah Williams Library (1963)

Brookings

South Dakota State University H. M. Briggs Library (1889)

Pierre

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)

Sioux Falls

Augustana College Mikkelsen Library (1969)
Sioux Falls Public Library (1903)

Spearfish

Black Hills State College Library Learning Center (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 Jere Whitson Memorial Library (1969)

Jackson

Lambuth College Luther L. Gobbel Library (1967)

Jefferson City

Carson-Newman College 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 James D. Hoskins Library (1907)
University of Tennessee Law Library (1971)

Martin

University of Tennessee at Martin Paul Meek Library (1957)

Memphis

Mamphis-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 Law Library (1976)

Tennessee State Library and Archives (unknown)

Tennessee State University Brown-Daniel Library (1972)

Vanderbilt University Alynne Queener Massey Law Library (1976)

Vanderbilt University Library (1884)

Sewanee

University of the South Jessie Ball duPont Library (1873)

TEXAS

Abilene

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-Castañeda 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 David 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 Gaston T. Gooch Library (1965)

Dallas

Bishop College Zale Library (1966)

Dallas Baptist University Vance Memorial Library (1967)

Dallas Public Library (1900)

Southern Methodist University Fondren Library (1925)

University of Texas Health Science Center-Dallas Library (1975)

Denton

North Texas State University Library (1948)

Edinburg

Pan American University Library (1959)

El Paso

El Paso Public Library (1906)

University of Texas at El Paso Library Documents & Maps Library (1966)

Fort Worth

Fort Worth Public Library (1905)

Texas Christian University Mary Coats Burnett Library (1916)

Galveston

Rosenberg Library (1909)

Houston

Houston Public Library (1884)

North Harris County College Learning Resource Center (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 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. Yearly Library (1970)

Longview

Nicholson Memorial Public Library (1961)

Lubbock

Texas Tech University Library (1935) REGIONAL

Texas Tech University School of Law Library (1978)

Marshall

Wiley College Thomas Winston Cole Sr. Library (1962)

Nacogdoches

Stephen F. Austin State University Steen Library (1965)

Plainview

Wayland Baptist University Van Howeling Memorial Library (1963)

Richardson

University of Texas at Dallas McDermott Library (1972)

San Angelo

Angelo State University Porter Henderson Library (1964)

San Antonio

Saint Mary's University Academic Library (1964)

Saint Mary's University 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 Arthur Hopkins Library (1963)

Texarkana

Texarkana Community College Palmer Memorial Library (1963)

Victoria

Victoria College/University of Houston Victoria Campus Library (1973)

Waco

Baylor University 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)

Ephraim

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)

Montpelier

Vermont Department of Libraries (1845)

Northfield

Norwich University Library (1908)

South Royalton

Vermont Law School Library (1978)

VIRGIN ISLANDS

Saint Croix

Florence Williams Public Library (1968)

Saint Thomas

College of the Virgin Islands Ralph M. Paiewonsky Library (1973)
Enid M. Baa Library and Archives (1968)

VIRGINIA

Alexandria

Dept. of the Navy Office of Judge Advocate General Law Library (1963)

Arlington

George Mason University School of Law Library (1981)

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 E. Lee Trinkle Library (1940)

Hampden-Sydney

Hampden-Sydney College Eggleston Library (1891)

Hampton

Hampton Institute Huntington Memorial Library (1977)

Harrisonburg

James Madison University Carrier Library (1973)

Hollins College

Hollins College Fishburn Library (1967)

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 Library (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 MCDEC 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 James Branch Cabell Library (1971)
Virginia State Law Library (1973)
Virginia State Library (unknown)

Salem

Roanoke College Library (1886)

Williamsburg

College of William and Mary Marshall-Wythe Law Library (1978)
College of William and Mary Swem Library (1936)

Wise

Clinch Valley College John Cook Wyllie Library (1971)

WASHINGTON

Bellingham

Western Washington University Mable Zoe Wilson Library (1963)

Cheney

Eastern Washington University JFK Library (1966)

Ellensburg

Central Washington University Library (1962)

Everett

Everett Public Library (1914)

Midway

Highline Community College Library (1983)

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

Seattle

Seattle Public Library (1908)

University of Washington Suzallo 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 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)

Glenville

Glenville State College Robert F. Kidd Library (1966)

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 College Library (1921)

Shepherdstown

Shepherd College Ruth Scarborough Library (1971)

Weirton

Mary H. Weir Public Library (1963)

WISCONSIN

Appleton

Lawrence University Seeley G. Mudd Library (1869)

Beloit

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 Learning Resources Center (1968)

La Crosse

La Crosse Public Library (1883)

University of Wisconsin-La Crosse Murphy Library (1965)

Madison

Madison Public Library (1965)

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

Alverno College Library/Media Center (1971)

Medical College of Wisconsin, Inc. Todd Wehr Library (1980)

Milwaukee County Law and Reference Library (1934)

Milwaukee Public Library (1861) REGIONAL

Mount Mary College Haggerty Library (1964)

University of Wisconsin-Milwaukee Library (1960)

Oshkosh

University of Wisconsin-Oshkosh Forrest R. Polk Library (1956)

Platteville

University of Wisconsin-Platteville Karrmann Library (1964)

Racine

Racine Public Library (1898)

Ripon

Ripon College Library (1982)

River Falls

University of Wisconsin-River Falls Chalmer Davee Library (1962)

Sheboygan

Mead Public Library (1983)

Stevens Point

University of Wisconsin-Stevens Point Learning Resources Center (1951)

Superior

Superior Public Library (1908)

University of Wisconsin-Superior Jim Dan Hill Library (1935)

Waukesha

Waukesha Public Library (1966)

Wausau

Marathon County Public Library (1971)

Whitewater

University of Wisconsin-Whitewater Harold Anderson Library (1963)

WYOMING

Casper

Natrona County Public Library (1929)

Cheyenne

Wyoming State Law Library (1977)

Wyoming State Library (unknown) REGIONAL

Gillette

Campbell County Public Library (1980)

Laramie

University of Wyoming, Coe Library (1907)

University of Wyoming Law Library (1978)

Powell

Northwest Community College John Taggart Hinckley Library (1967)

Riverton

Central Wyoming College Library (1969)

Rock Springs

Western Wyoming Community College Library (1969)

Sheridan

Sheridan College, Griffith Memorial Library (1963)

APPENDIX B

List of District Offices of the U.S. Department of Commerce

ALABAMA

***Birmingham**—2015 2nd Ave. North, 3rd Floor Berry Bldg., 35203, Area Code 205 Tel 264-1331, FTS 229-1331

ALASKA

Anchorage—701 C Street, P.O. Box 32, 99513, Area Code 907 Tel 271-5041, FTS 8 907 271-5041

ARIZONA

Phoenix—Federal Bldg. & U.S. Courthouse, 230 N. 1st Avenue, Room 3412, 85205, Area Code 205 Tel 254-3285, FTS 261-3285

ARKANSAS

Little Rock—Suite 311, Savers Federal Building, 320 W. Capitol Avenue, 72201, Area Code 501 Tel 378-5794, FTS 740-5794

CALIFORNIA

Los Angeles—Room 800, 11777 San Vicente Boulevard, 90049, Area Code 213 Tel 209-6707, FTS 793-6707

•**Santa Ana**—116-A W. 4th Street, Suite #1, 92701, Area Code 714 Tel 836-2461, FTS 799-2461

•**San Diego**—6363 Greenwich Drive, 92122, Area Code 619 Tel 293-5395, FTS 895-5395

•**San Francisco**—Federal Building, Box 36013, 450 Golden Gate Avenue, 94102, Area Code 415 Tel 556-5860, FTS 556-5868

COLORADO

***Denver**—Room 119, U.S. Customhouse, 721-19th Street, 80202, Area Code 303 Tel 844-3246, FTS 564-3246

CONNECTICUT

***Hartford**—Room 610-B, Federal Office Building, 450 Main Street, 06103, Area Code 203 Tel 722-3530, FTS 244-3530

DELAWARE

Serviced by Philadelphia District Office

DISTRICT OF COLUMBIA

Serviced by Baltimore District Office

FLORIDA

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