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Semiconductor Measurement Technology:

A Software Program for Aiding the Analysis of Ellipsometric Measurements, Simple Spectroscopic Models

J. F. Marchiano

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J. F. Marchiando

Semiconductor Electronics Division
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Semiconductor Measurement Technology:
**A Software Program for Aiding the
Analysis of Ellipsometric Measurements,
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MAIN2 is a software program for analyzing spectroscopic ellipsometric measurements. MAIN2 consists mainly of subroutines written in FORTRAN that are used to invert the standard reflection ellipsometry equations for simple systems. Here, a system is said to be simple if the solid material sample is characterized by models which assume at least the following: (1) materials are nonmagnetic; (2) samples exhibit depth-dependent optical properties, such as one with layered or laminar structure atop a substrate that behaves like a semi-infinite half-space; (3) layers are flat and of uniform thickness; and (4) the optical medium within each ambient/layer/substrate is isotropic, homogeneous, local, and linear. The ambient region refers to that region of space which lies external to the layer/substrate structure of the sample. Usually, the ambient region involves a medium of air or vacuum. Each layer is characterized by a thickness and a dielectric function. The dielectric function of a region, i.e., ambient, layer, or substrate, is represented by the Bruggeman effective medium approximation (EMA). Within the EMA, the effective medium of a region is characterized by an aggregate mixture of constituent media, and the dielectric function of each constituent medium is known a priori. The constituent dielectric functions are taken from the literature. The ellipsometric equations are formulated as a standard damped nonlinear least-squares problem and then solved by an iterative method when possible. The program is sufficiently modular to allow one to modify some of the models used in the calculations.

Key words: ellipsometry; EMA; FORTRAN; modeling; software; spectroscopic models.

1. Introduction

In general, when linearly polarized light is incident on a flat surface, it becomes elliptically polarized upon reflection. Ellipsometry involves measuring this induced change in polarization, as well as understanding the measured change in polarization in terms of the optical properties of the material medium. The optical properties of the medium are characterized by the dielectric function and its spatial distribution. MAIN2 is a program for analyzing ellipsometric measurements to find the dielectric function and its spatial distribution. MAIN2 consists mainly of FORTRAN* subroutines that are used to invert a standard set of reflection ellipsometry equations. The systems under consideration here involve only simple structures such as those containing flat, thin, solid films atop a substrate.

A system is said to be simple if the solid material sample may be characterized by models that include at least the following: (1) materials are nonmagnetic; (2) samples exhibit depth-dependent optical properties, e.g., one with a layered or laminar structure atop a substrate that behaves like a semi-infinite half-space; (3) layers are flat and of uniform thickness; and (4) the optical medium within each ambient/layer/substrate is isotropic, homogeneous, local, and linear. The ambient region refers to that region of space which lies external to the layer/substrate structure of the sample. Usually, the medium of the ambient region is air or vacuum. The use of these assumptions is well documented [1-9].

The models used here involve at least two kinds of parameters: each layer is characterized in part by a thickness, and the dielectric function of the medium is expressed in terms of the effective medium approximation (EMA) due to Bruggeman [10-13]. The optical behavior of the ambient, layer, or substrate region is characterized as a macroscopic or physical aggregate mixture of constituent media where the dielectric function of each constituent medium is assumed to be known a priori, and the physical size or cross section of any given aggregate is much smaller than the classical wavelength of the incident light.

* Disclaimer: Certain commercial equipment, instruments, materials, or software products are identified by name in this document in order to adequately specify the experimental procedure or software development. Such identification does not imply recommendation or endorsement by the National Institute of Standards and Technology, nor does it imply that the materials, equipment, or software products identified are necessarily the best available for the intended purpose.

Here, the dielectric functions of the constituent media serve as basis functions in representing the effective dielectric function of the spatial region. The relative amount that each constituent medium contributes in representing the effective medium is given by a scalar coefficient and is called a volume fraction. The effective dielectric function is expressed in terms of dielectric functions and volume fractions of the constituents.

A limited database of the characteristics of the constituent media is stored in files, see section 6.5 [4]. These files usually contain a profile of the dielectric function, e.g., a point function over a range of discrete photon energies. Each of these data files has its own distinct subroutine in the software program to interpret the format of stored data. The convention associated with naming these subroutines and data files allows one to easily increase the number and/or resolution of the databases. Also, some provision is made for passing parameters to these subroutines, so that one may alter or change the models used in the representation of the dielectric function.

With only three kinds of model parameters to characterize a region, a sample may be assembled layer by layer atop a substrate. Since the natural parameters of the formulation involve only thickness and dielectric function, it is straightforward to analyze several distinct samples collectively. Here, the program is said to have a multiple-sample capability.

Because of the method of indexing the parameters used in the program, it is possible for two distinct regions to have a model parameter in common, e.g., a common dielectric function but a distinct thickness. Also, it is possible for distinct samples to have parameters in common. Such cases may arise when analyzing samples which have undergone some type of limited processing, e.g., changes in thickness due to etching. Here, the program is said to allow coupling between samples and layers.

The phenomenological models and methods of solution are classical. The ellipsometric equations are formulated as a standard nonlinear, damped least-squares problem that is solved by an iterative method [14–17]. Following the convergence (or nonconvergence) of the iterations to a *good* solution, i.e., within the resolution of the measurement by the instrumentation, the program stops.

Regarding the uniqueness of the calculated solution that is found by minimizing a residual in the least-squares sense, it is important to realize that multiple local minima (pseudo

solutions) may exist, as well as correlation among the modeling parameters [18-21]. Although the program serves as a tool in finding solutions at local minima, the responsibility of assessing the consistency and appropriateness of the resulting solution remains entirely dependent on the user. Because it is possible for the number of model parameters to become large and the run times to become long, the program was designed to run in batch mode, as opposed to interactive mode. Regarding the calculation of the uncertainty of the model parameters, the program uses the LINPACK library [15], which is public domain software.

Although no graphic displays are provided while running the program, provision is made for selecting specific sets of data for output. These data are written to a file in a format amenable to the generation of graphics later. Thus, graphics capability is dependent upon the resource library available at the local computing site. Actually, any one of several software graphics packages would be more than adequate. But for convenience, as well as for completeness, this document refers to the NCAR software graphics package [22, 23]. This is mentioned briefly in section 4.1.3.

This report presents a brief overview of the theory and methods of solution and provides a brief manual of operations or guide for the user to the options and capabilities of the software program. Section 2 discusses the models of the dielectric functions. Section 3 discusses the methods of inverting the ellipsometric equations. Section 4 discusses the manual of operations for the software package. This includes an overview regarding some of the considerations that went into the design of the software package. This overview includes a short listing of parameters which are used in specifying the allocations of the various arrays. Presented next are the free-field formats which are used when entering the required sets of input data. These include the tabular lists of model parameters, the specification or characterization of the samples, and the collective sets of measurements of the ellipsometric angles. Finally, information is given regarding the command options that are available to the user for exercising operational control over the program, i.e., constraints of procedures during analyses. Section 5 discusses a few selected examples of actual runs of the software package. The input and output data files are listed. Section 6 contains a listing of the software source files. Lastly, the appendix contains a quick reference guide for using the program and building the necessary input data files.

The source code is written predominantly in standard FORTRAN-77. Minor compiler extensions involve the DO-ENDDO, the INCLUDE, and the OPEN and CLOSE statements; such are appropriate for a VAX computer. The system clock is also machine dependent, see section 6.3.12. The source code contains some in-line comments for the user's convenience, but some compilers may find this to be a nuisance. The more expert user may want to modify some of the routines while taking advantage of the interior data structure of the program, whereas the less expert user may simply want to operate the package as presented. A copy of the ASCII files of the source program and an installation guide are available from the author upon written request on letterhead stationery and receipt of a DOS-formatted floppy diskette or a small reel of nine-track magnetic tape.

2. The Dielectric Function

The theory describing the scattering of light for ellipsometry, as well as the numerical methods of calculation of the models, has been discussed in detail elsewhere [1-3]. The discussion presented in [3] involved the reflection and refraction of a time-harmonic monochromatic plane electromagnetic wave obliquely-incident on a flat plane surface of a stratified medium exhibiting depth-dependent optical properties. The optical properties of the material medium were assumed to be piecewise continuous, isotropic, local, linear, and not perturbed by the effects of free charges and surface currents.

The coordinate geometry used here is the same as that presented in [3]. The material medium is assumed to occupy the semi-infinite positive half-space ($z > 0$) with the flat surface being the plane ($z = 0$). For the isotropic homogeneous medium with depth-dependent (z) optical properties, there is translational invariance within the (x, y) plane. The z -axis is aligned in a direction normal to the surface and planes of stratification. A lossless isotropic homogeneous medium like air or vacuum is assumed to occupy the so-called ambient region ($z < 0$). A source time-harmonic monochromatic plane wave is assumed to be incident on the surface of the medium ($z = 0$), from the ambient region ($z < 0$), in a direction of angle ϕ with respect to the surface normal. The plane of incidence is taken to be the (z, x) plane, and the direction cosines of propagation are both positive.

The profile of the stratified structure of the dielectric function is approximated by a stepped profile; the dielectric function of a region, i.e., ambient, layer, or substrate, is assumed to depend only on the optical frequency of light. The dielectric function in [3] was expressed in terms of one index of refraction and one extinction coefficient per optical frequency. Although this may be adequate for analyzing measurements involving very few optical frequencies, spectroscopic ellipsometry usually involves analyzing measurements at very many frequencies. Here, dispersion is used to advantage in analysis; i.e., the dielectric function may change with frequency, whereas the layer thickness may not change. The dielectric function of the ambient, layer, or substrate region is assumed to be characterized by the optical behavior of a macroscopic or physical aggregate mixture of constituent media, where the dielectric function of each constituent medium is known a priori. Further, the cross-sectional diameter of any given aggregate is assumed to be small compared to the classical wavelength of the incident light, and there is negligible interaction between

neighboring aggregates. Such ideas in part form bases of several effective medium theories. The model assumed here is the effective medium approximation (EMA) associated with Bruggeman [10–13]. The relative amount that each constituent medium contributes to the effective medium of the region is given by a real-valued scalar number called a volume fraction. The following subsections present brief discussions regarding the calculations of the dielectric functions of the constituent media, the effective media within the EMA, and the partial derivatives of the dielectric functions with respect to the associated model parameters.

2.1 Constituent Media

Within any given region, i.e., ambient, layer, or substrate, the effective medium is assumed to behave like an aggregate mixture of distinct constituent media. Within the EMA, the dielectric function (ϵ) of the effective medium is expressed in terms of the dielectric functions (ϵ_j) of the constituent media, where j indexes the distinct constituent media. The (ϵ_j) serve as basis functions for (ϵ) and are assumed to be known functions of the optical frequency.

Here, a constituent medium is characterized by its optical properties, i.e., the dielectric function. A constituent medium is considered distinct insofar as its optical dielectric function is distinct. Hence, a constituent medium may refer to a distinct chemical entity and its associated optical properties, e.g., due to a phase state. For example, regarding a thermally grown oxide atop a silicon wafer, j may refer to the distinct chemical entities of SiO_2 or Si, as well as the associated phases that may be present, e.g., amorphous SiO_2 , amorphous Si, or crystalline Si. Since these materials have distinct dielectric functions, they are considered to be three distinct constituent media.

To calculate the dielectric function of a constituent medium, a distinct subroutine is used for each distinct constituent medium. Each of these subroutines contain an argument list, so that it is possible to optimize on model parameters that are local to the individual constituent dielectric function. Since these dedicated subroutines have similar names and argument lists, one may easily modify the database of any individual constituent medium. The convention used here for naming subroutines that calculate constituent dielectric functions is of the form, DIELxx, where xx refers to a two-digit number between 01 and 99.

These subroutines calculate (ϵ_j) from those models that have been found or reported in the available open literature. Usually, this involves evaluating a Sellmeier equation or a spline fit of a point function defined on a discrete grid of energies, i.e., where the optical frequencies have been expressed in terms of energy. The point function is stored in and read from some data file, and the spline-fitting algorithms are from the GAMS software library [14]. The point functions are stored in files with suggestive filenames. For example, to calculate the dielectric function of gallium arsenide, the subroutine DIEL08 reads and stores the entire point function that is stored in file W.GA_AS during the first call, see sections 6.5.8 and 6.6.6, respectively. Then, DIEL08 needs to evaluate only two spline fits per call, i.e., the real and imaginary parts of the complex refractive index or dielectric function.

Note also that these subroutines, i.e., DIELxx, are all called from the same subroutine, DIELMN, see section 6.4.4. (LMN is meant to be a mnemonic for *elements*.) If it is ever decided (by the user) that the number of distinct constituent media in the database is to be enlarged by including additional subroutines, then appropriate calls to these additional subroutines must be included in the subroutine DIELMN. Further, it may be necessary to modify the parameter called `nlmnts` that is discussed in section 4.1.2 as well.

2.2 The Effective Medium Approximation

The effective medium approximation [10–13] for determining the dielectric function (ϵ) of a distinct spatial region, i.e., ambient, layer, or substrate, is given by the following equation

$$0 = \sum_{j=1}^N f_j \left(\frac{\epsilon_j - \epsilon}{\epsilon_j + 2\epsilon} \right) \quad (1)$$

subject to the constraint

$$\sum_{j=1}^N f_j = 1, \quad (2)$$

where N denotes the number of distinct constituent media in the mixture, f_j denotes the volume fraction of the j^{th} constituent, ϵ_j denotes the dielectric function of the j^{th} distinct constituent medium evaluated at the appropriate classical optical frequency of light, and ϵ is the dielectric function of the effective medium. It is assumed that f_j and ϵ_j are known on input, and that f_j is independent of the frequency and is a real valued scalar. Equation (1) must then be solved for ϵ . The method of solution used here is Newton iteration. This involves a three-step procedure.

The first step involves reformulating eq (1) in order to simplify the functional dependence on ε . Equation (1) may be written as

$$0 = \sum_{j=1}^N f_j \left\{ \frac{\varepsilon_j + 2\varepsilon - 3\varepsilon}{\varepsilon_j + 2\varepsilon} \right\} = \sum_{j=1}^N f_j \left\{ 1 - \frac{3\varepsilon}{\varepsilon_j + 2\varepsilon} \right\}.$$

Thus,

$$\frac{1}{3\varepsilon} = \sum_{j=1}^N \frac{f_j}{\varepsilon_j + 2\varepsilon}. \quad (3)$$

Equation (1) may also be written as

$$\sum_{j=1}^N f_j \frac{\varepsilon_j}{\varepsilon_j + 2\varepsilon} = \varepsilon \sum_{j=1}^N \frac{f_j}{\varepsilon_j + 2\varepsilon} = \varepsilon \left(\frac{1}{3\varepsilon} \right) = \frac{1}{3}, \quad (4)$$

where a substitution has been made from eq (3).

The second step involves applying the Newton algorithm to eq (4). Here, one seeks the root to an equation, say Q , given by

$$Q(\varepsilon) = \sum_{j=1}^N \frac{f_j \varepsilon_j}{(\varepsilon_j + 2\varepsilon)} - \frac{1}{3}. \quad (5)$$

The root minimizes $|Q|$. The variation of Q given by

$$\delta Q = -(\delta\varepsilon) 2 \sum_{j=1}^N \frac{f_j \varepsilon_j}{(\varepsilon_j + 2\varepsilon)^2} \quad (6)$$

forms the basis for the Newton step. The Newton step is related to $(Q/\delta Q)$.

The third step involves providing a reasonable initial solution. This is necessary for starting any iterative method of solution. For convenience, the initial solution is given by

$$\varepsilon = \frac{1}{3} (2\varepsilon_{\parallel} + \varepsilon_{\perp}),$$

where

$$\varepsilon_{\parallel} = \sum_{j=1}^N f_j \varepsilon_j \quad \text{and} \quad \frac{1}{\varepsilon_{\perp}} = \sum_{j=1}^N \frac{f_j}{\varepsilon_j},$$

which follows from considering two extreme cases when the electric field vector is oriented either parallel or perpendicular to the layers of the stratified media.

The criterion for convergence in finding the root is that the Newton step be at least six orders of magnitude smaller than the magnitude of the dielectric function of the effective medium. This algorithm is located in subroutine DIEEMA, see section 6.4.2.

To help understand eqs (1) and (5), consider the following example. Consider a sample of silicon with a thermally-grown oxide layer. Let the layered structure consist of two layers and a substrate. Here, the substrate is silicon, and the top layer is amorphous SiO_2 . Let a transition region layer lie between the top layer and substrate, and let it be an aggregate mixture of half Si and half amorphous SiO_2 . This structure involves three effective media, i.e., one to a region, but only two constituent media, i.e., crystalline Si and amorphous SiO_2 . Accordingly, (ϵ_j) may refer to either (ϵ_{Si}) or $(\epsilon_{\text{SiO}_2})$. Regarding eq (5), it follows that $(N = 1)$ and $(f_j = 1)$ for both the top layer and the substrate regions. Hence, $(\epsilon = \epsilon_{\text{SiO}_2})$ for the top layer, and $(\epsilon = \epsilon_{\text{Si}})$ for the substrate. Regarding the transition region, $(N = 2)$ and $(f_{\text{Si}} = f_{\text{SiO}_2} = 0.5)$. Letting the optical frequency be that corresponding to an energy of 2.0 eV, one may evaluate the complex dielectric functions for the constituent media. From sections 2.1, 6.6.1, and 6.6.3, it follows that

$$\epsilon_{\text{Si}} \approx 15.256 + i 0.172 \quad \text{and} \quad \epsilon_{\text{SiO}_2} \approx 2.124 + i 0.0,$$

where $i = \sqrt{-1}$. Then, regarding eq (5), the root is found to be

$$\epsilon \approx 6.747 + i 0.052,$$

i.e., the dielectric function of the effective medium of the transition region.

2.3 Partial Derivatives

The problem associated with inverting a standard set of reflection ellipsometry equations has been discussed in detail elsewhere [1-3]. The inverse problem is formulated as a least-squares problem. The method of solution used here involves an iterative procedure for improving the numerical values of the model parameters [3]. This requires some understanding of the functional dependence of the dielectric function on the necessary model parameters. Hence, one must calculate the partial derivatives of the dielectric function with respect to any model parameter that may be selected for optimization. Regarding the EMA, this involves at least two kinds of partial derivatives.

The first kind involves variations in model parameters that are local to the constituent dielectric function, but yet are independent of volume fraction and thickness. Letting the prime denote a partial derivative with respect to such a model parameter, and then operating on eq (4), it follows that

$$0 = \sum_{j=1}^N f_j \left\{ \frac{\epsilon'_j}{(\epsilon_j + 2\epsilon)} - \frac{\epsilon_j \epsilon'_j}{(\epsilon_j + 2\epsilon)^2} - \frac{2\epsilon_j \epsilon'}{(\epsilon_j + 2\epsilon)^2} \right\},$$

which may be rearranged to yield

$$\epsilon' = \epsilon \frac{\sum_{j=1}^N \frac{f_j \epsilon'_j}{(\epsilon_j + 2\epsilon)^2}}{\sum_{i=1}^N \frac{f_i \epsilon_i}{(\epsilon_i + 2\epsilon)^2}}. \quad (7)$$

To evaluate ϵ' from eq (7), the program uses subroutine DIEMAD, see section 6.4.3.

The second kind involves variations in the volume fractions. Again, starting with eq (4), it follows that

$$0 = \sum_{j=1}^N \left(\frac{\epsilon_j}{\epsilon_j + 2\epsilon} \right) (\delta f_j) - (\delta \epsilon) 2 \sum_{j=1}^N \frac{f_j \epsilon_j}{(\epsilon_j + 2\epsilon)^2},$$

which implies that

$$\left(\frac{\partial \epsilon}{\partial f_j} \right) = \frac{\left(\frac{\epsilon_j}{\epsilon_j + 2\epsilon} \right)}{2 \sum_{i=1}^N \frac{f_i \epsilon_i}{(\epsilon_i + 2\epsilon)^2}} \quad (8)$$

when the f_j are mutually independent variables. Yet, from eq (2), it follows that

$$0 = \sum_{j=1}^N (\delta f_j). \quad (9)$$

Hence, the variations are linearly dependent. Since each independent constraint removes one degree of freedom, if some of the volume fractions of a layer are selected for optimization, then at least two or more of the f_j must be involved in the variation. Since,

$$\delta \epsilon = \sum_{j=1}^N \left(\frac{\partial \epsilon}{\partial f_j} \right) \delta f_j,$$

then one may evaluate the partial derivative of ϵ with respect to a set of unconstrained variables ($\hat{f}_j$) by letting

$$\left(\frac{\partial \epsilon}{\partial \hat{f}_j} \right) = \left(\frac{\partial \epsilon}{\partial f_j} \right) - \left(\frac{\partial \epsilon}{\partial f_k} \right), \quad (10)$$

where j and k involve the set of model parameters that are selected for variation but are coupled by the constraint, where k involves a fixed index selected arbitrarily by the user, and where ($j \neq k$). For convenience, the program uses: ($k < j$). To evaluate the $(\partial \epsilon / \partial f_j)$ in eq (8), the software program uses subroutine DIEEMA, see section 6.4.2.

3. The Inverse Problem

3.1 Formulation of the Least-Squares Problem

In order to characterize the layered structure of the sample, it is necessary to invert the standard ellipsometric equations. These equations relate how the optical properties of the material sample induce a phase-shift in the reflected light that is measured by the ellipsometer. Because of the nonlinearity of the equations, it is usually not possible to find simple analytic expressions which will invert the equations. The common approach to performing such inversions is to formulate them as nonlinear least-squares problems [1–3]. Here, one considers a sequence of forward problems, where each increment of the sequence involves three distinct steps. The steps are: starting with a good estimate of values of the model parameters, determining the deviations between the experiment and the model, and then updating the model parameters with *better* values. This sequence is repeated until the magnitude of the corrections become sufficiently *small*.

The ellipsometric equations for the ellipsometric angles, Δ and ψ , are of the form:

$$\Delta = \Delta(\nu, \phi, \mathbf{b}) \quad \text{and} \quad \psi = \psi(\nu, \phi, \mathbf{b})$$

where ν is the frequency of the incident light; ϕ is the angle of incidence; and $\mathbf{b}$ is an array where the components specify the model parameters, e.g., layer thicknesses and volume fractions. The standard procedure for inverting the above equations involves minimizing some objective function or nonnegative scalar error expression containing the deviations between experiment and model of Δ and ψ in the least-squares sense, e.g.,

$$\begin{aligned} G(\mathbf{b}) &= \frac{1}{2M} \sum_{i=1}^M \left[\left(\frac{\Delta_i^e - \Delta_i^m}{\delta \Delta_i^e} \right)^2 + \left(\frac{\psi_i^e - \psi_i^m}{\delta \psi_i^e} \right)^2 \right] \\ &= \sum_{i=1}^M (g_{\Delta,i}^2 + g_{\psi,i}^2) = \mathbf{g}^T \mathbf{g} = |\mathbf{g}|^2 \end{aligned} \quad (11)$$

where superscripts (e, m) refer to experiment and model, respectively, M refers to the number of measurements of (Δ, ψ) from experiment, $\mathbf{g}$ is an array of the deviations, e.g., $(\Delta_i^e - \Delta_i^m)$, that are scaled by the uncertainties in the measurement, i.e.,

$$g_{\Delta,i} = \frac{1}{\sqrt{2M}} \left(\frac{\Delta_i^e - \Delta_i^m}{\delta \Delta_i^e} \right) = \mathbf{g}_{2i-1} \quad (12)$$

$$g_{\psi,i} = \frac{1}{\sqrt{2M}} \left(\frac{\psi_i^e - \psi_i^m}{\delta \psi_i^e} \right) = \mathbf{g}_{2i} \quad (13)$$

where $(1 \leq i \leq M)$, the superscript T denotes transposition, and the uncertainties in the measurement of Δ_i^ξ and ψ_i^ξ are denoted by $\delta\Delta_i^\xi$ and $\delta\psi_i^\xi$, respectively.

The third step of the sequence is concerned with the procedure for obtaining *better* numerical values for the model parameters, i.e., the Newton step. An estimate of the necessary correction may be realized by linearizing the functional representation of the model and solving the resulting matrix equation, $\mathbf{g} = \mathbf{J}\mathbf{v}$, where $\mathbf{v}$ is a column array (Newton step) for improving the model parameters that were selected to undergo variation, i.e., $v_j \propto \delta b_j$, and where the Jacobian $\mathbf{J}$ is a sparse matrix, $J_{ij} \propto (\partial\Delta_i/\partial b_j)$.

Such matrix equations are common to optimization problems. It is well known that additional numerical stability may result if one requests that the norm of $\mathbf{v}$ be minimized as well. This involves modifying the error expression to

$$G = (\mathbf{g} - \mathbf{J}\mathbf{v})^T(\mathbf{g} - \mathbf{J}\mathbf{v}) + \kappa\mathbf{v}^T\mathbf{v}, \quad (14)$$

where κ is a positive scalar parameter subjectively chosen between 0.01 and 1.0 for our calculations. Of course, the final solution $\mathbf{v}$ ought to be independent of κ .

It is also known that the columnar scaling of $\mathbf{J}$ affects the accuracy of the solution, as well as the effectiveness of κ . A simple choice for the scaling can be found by considering the diagonal elements from $\mathbf{J}^T\mathbf{J}$ and then defining the diagonal matrix, $\mathbf{S}$, where

$$S_{jj} = \left([\mathbf{J}^T\mathbf{J}]_{jj} \right)^{1/2}. \quad (15)$$

Letting

$$\begin{aligned} \tilde{\mathbf{J}} &= \mathbf{J}\mathbf{S}^{-1}, \\ \tilde{\mathbf{v}} &= \mathbf{S}\mathbf{v}, \\ \mathbf{r} &= \mathbf{g} - \mathbf{J}\mathbf{v} = \mathbf{g} - \tilde{\mathbf{J}}\tilde{\mathbf{v}}, \end{aligned}$$

a suitable error expression may be defined by

$$\begin{aligned} G &= (\mathbf{g} - \tilde{\mathbf{J}}\tilde{\mathbf{v}})^T(\mathbf{g} - \tilde{\mathbf{J}}\tilde{\mathbf{v}}) + \kappa\tilde{\mathbf{v}}^T\tilde{\mathbf{v}} \\ &= \mathbf{r}^T\mathbf{r} + \kappa\tilde{\mathbf{v}}^T\tilde{\mathbf{v}}. \end{aligned} \quad (16)$$

The criterion for critical points or relative minima is a vanishing variation, i.e., $\partial G/\partial \tilde{v}_j = 0$, which yields a set of equations that may be expressed as

$$\begin{bmatrix} \mathbf{1} & \tilde{\mathbf{J}} \\ \tilde{\mathbf{J}}^T & -\kappa \mathbf{1} \end{bmatrix} \begin{bmatrix} \mathbf{r} \\ \tilde{\mathbf{v}} \end{bmatrix} = \begin{bmatrix} \mathbf{g} \\ \mathbf{0} \end{bmatrix},$$

and must then be solved for $\tilde{\mathbf{v}}$.

Because of the sparsity of the Jacobian, it is expedient to utilize an iterative method for solving the above matrix algebra problem. Algorithms [14, 15] exist that specifically address this type of problem, one [16, 17] of which utilizes a relatively stable Lanczos process (Krylov space decomposition) in formulating the method of steepest-descents. Essentially, the method requires that each updating vector be orthogonal to the previous update vectors. From this procedure, one finds $\tilde{\mathbf{v}}$, which leads to $\mathbf{v}$, which is then used to improve the estimate of the values for the model parameters, e.g., $b_j^{\text{new}} = b_j^{\text{old}} + v_j$.

Using this improved $\mathbf{b}$, the sequence is repeated again until either: $|\mathbf{g}|$ becomes sufficiently *small*, of the order of a few millidegrees, e.g., the resolution of the measurement, or until $|\tilde{\mathbf{v}}|$ become sufficiently *small* so that $|\mathbf{g}|$ suffers no further reduction regardless of magnitude. It is especially during this last case that it becomes necessary to scan a grid of model parameters. Multiple local-minima may be encountered, e.g., nonuniqueness. Often, this reveals either: (i) correlation which prevents model parameters from being resolved independently; i.e., the measurement data are not sufficiently functionally independent which thereby induces a functional dependence among the model parameters; or (ii) the inadequacy of the model in providing a sufficiently good physical description of the process, which is likely whenever $|\mathbf{g}|$ greatly exceeds the resolution of the measurements.

Finally, it is important to realize that in the above-outlined steps, the emphasis centers on searching for and ascribing *good* values to the parameters of a physical model which has already been specified. Only one specific model is assumed to have been applied to a given set of measurements. But often situations may occur, or questions may arise, where it is important to consider alternative models during the effort to further reduce the value of the error expression G , and these must be investigated as well. Also, it is possible that two or more distinct models may be found that reduce the deviations in $|\mathbf{g}|$ to comparable magnitudes. Then, the problem of characterizing the sample becomes one of comparing models which ought to lead toward a decision about selecting the *better* model. One heuristic approach has been to select that model which provides the smallest deviations,

i.e., $|g|$, while utilizing the fewest modeling parameters and being consistent with physical reality. However, comparisons assume some criteria or ordering, and that requires a number. So the problem becomes one of reducing a model to a number. This reduction is certainly not simple and fully merits its own discussion, e.g., hypothesis testing and decision theory. But such a discussion is beyond the scope that is intended here, so that it is expedient to direct the reader to consider simple statistics and use the F -statistic in assessing the so-called *goodness-of-fit* test. For further discussion on topics such as parameter estimation, hypothesis testing, significance testing, and other formulations involving decision processes, the reader is advised to consider the statistics literature available.

3.2 Sensitivity Analysis of Model Parameters

In the above discussion of the least-squares problem, the emphasis was on obtaining accurate numerical values for the model parameters. Following this, it is natural to consider next some assessment of the uncertainties associated with those values. For a restricted class of linearizable problems and assumptions, one may ascribe estimates to these uncertainties by utilizing a formulism similar to that used in the least-squares problem [3].

Starting with the functional representation of the model, and then expanding about the critical or fixed point solution, the deviations may be expressed by assuming variations out to first order, i.e.,

$$\Delta_i^c - \Delta_i^m = \sum_{j=1}^N \left. \frac{\partial \Delta_i}{\partial b_j} \right|_o \delta b_j + \left. \frac{\partial \Delta_i}{\partial \phi} \right|_o \delta \phi + \tilde{e}_{\Delta,i} \quad (17)$$

and

$$\psi_i^c - \psi_i^m = \sum_{j=1}^N \left. \frac{\partial \psi_i}{\partial b_j} \right|_o \delta b_j + \left. \frac{\partial \psi_i}{\partial \phi} \right|_o \delta \phi + \tilde{e}_{\psi,i} \quad (18)$$

where N refers to the number of distinct model parameters, and $\tilde{e}_i$ refers to the uncertainty associated with individual measurements of (Δ, ψ) performed by the instrument. Further, it may be the case that during the course of analysis of finding the critical point solution, some of the model parameters will have had values and uncertainties assigned to them from some earlier experiment or measurement that is external to and distinct from those being analyzed here, e.g., values taken from the literature. These values are assumed as given and remain unchanged during the calculations. Consequently, the set of model parameters (δb_j) may be partitioned into two disjoint sets, those that remain unchanged

(u_j) and those that are allowed to vary (v_j) . This allows both of the above expansions to be combined and expressed as

$$g_i = J_{v,ij}v_j + J_{u,ij}u_j + J_{\phi,i}\tilde{\phi}_i + \tilde{e}_i, \quad (19)$$

where g_i refers to deviations in (Δ, ψ) between measurement and theory, e.g., $(\Delta_i^e - \Delta_i^m)$ without scaling by the measurement uncertainty; J refers to the Jacobian or the array of partial derivatives that is appropriate for the partitioning and evaluated at the critical point; and $\tilde{\phi}_i$ involves the uncertainty in the angle of incidence and the assumption of stochastic independence between each measurement, and the implied summation affects only the j index. The sensitivity analysis of the model parameters centers on the procedure of assigning values to the uncertainty in (b_j) that are associated with (v_j) . Since this has been discussed in [3], only terms associated with (v_j) are considered in what follows.

From eqs (11), (14), and (19), it follows that the minimum value of the error expression G is attributed to residuals that are due to measurement uncertainties $\tilde{e}_i$ that are assumed to behave as random variables in a statistical sense, i.e., being stochastically independent and identically distributed. So, when G is evaluated at the critical point solution, it is assumed that

$$G_o = |\mathbf{g}|^2 = |\mathbf{e}|^2, \quad (20)$$

and that an expansion of G about the critical point may be shifted to zero and written as

$$\tilde{G} = G - G_o = |\mathbf{g} - \mathbf{J}_v \mathbf{v}|^2 - |\mathbf{g}|^2. \quad (21)$$

A simple estimate of the variances of the model parameters may be found from

$$\langle v_j v_k \rangle = s_g^2 \left[\left(\mathbf{J}_v^T \mathbf{J}_v \right)^{-1} \right]_{jk}, \quad (22)$$

where

$$s_g^2 = \frac{\mathbf{g}^T \mathbf{g}}{2M - N} \quad (23)$$

estimates the variance of a χ^2 distribution with $2M - N$ degrees of freedom, M is the number of measurements of (Δ, ψ) , and N is the number of model parameters (v_j) undergoing variation. In the absence of correlation, the magnitude of uncertainty $(\mathcal{U})$ assigned to model parameter (v_j) may be estimated by

$$\mathcal{U}(v_j) \leq \langle v_j v_j \rangle^{1/2}. \quad (24)$$

To calculate the necessary terms given in eq (22), the program uses subroutine CORLAT.

4. Manual of Operations

In order to use MAIN2, it is necessary to: (1) specify the model parameters that characterize the layered structure of the sample, (2) collect the necessary measurement data of ellipsometric angles and the associated energies and angles of the incident light, (3) assign size allocations of arrays which hold these data, (4) assign formats and filenames which are provided for entering the input data and receiving the output data from calculations, (5) understand the stored databases of constituent media, and (6) understand the limitations and capabilities of the software package and its utility for implementing strategies in analyzing the measurement data. The filename convention assumes a filename and an extension made of alphanumeric characters in the standard format given by: filename.extension. This section presents a brief overview of these considerations.

4.1 Software Development Considerations

The main program, MAIN, performs a small set of functions, see section 6.2.1. First, it calls a subroutine to open the necessary data files. Second, it requests a subroutine to read most of the input data file. Third, it allows the user to select an option from a menu or tabulated list of command options and then calls the appropriate subroutine. Following the return from the subroutine to the main program, the main program stops; no further command options are processed.

4.1.1 Input/Output Files

MAIN2 involves at least two kinds of data files. The first kind of file involves five input/output files for calculations. Two files serve for entering input data, and three files serve for collecting output data.

X.DAT is an input data file. It contains: the model parameters that characterize the sample, the configuration of the layered structure of the sample, and the ellipsometric angles of the measurement data. An example of an X.DAT file is shown in section 4.2.9.

X.INN is an input data file. It contains the sequential list of command options that provide control of the program. These are discussed further in section 4.3. Examples of X.INN files may be found in section 5.

X.OUT is an output data file. It contains a collective list of: all the entered input data and the general proceedings generated during the course of a calculation, as well as any informative error messages. Examples are shown in section 5.

X.SOUT is an output data file for intermediate solutions. It contains the breakpoint information that may be generated during any grid scan of the model parameters. This information is written to the file at periodic intervals of 15 CPU-minutes and overwrites the information from previous breakpoints, so that only the last or most recent breakpoint is retained. The procedure for restarting or resuming a previously interrupted calculation involves the simple task of appending the output of this file X.SOUT onto the end of file X.INN, i.e., without any intervening blank lines, and then re-executing the job. When the job is re-executed, the program will attempt to read only one set of breakpoint information in file X.INN before resuming calculations. Consequently, it is important to replace any earlier breakpoint data in X.INN, as appropriate.

X.PLOT is an output data file for graphics. The data are formatted in a manner that is intended to be amenable for later reading and plotting. Examples are shown in section 5.

These files are opened initially by subroutine FILEOP, see section 6.2.2. Since breakpointing involves opening/closing files, other open/close statements may be found in subroutines SCANO1 and SCANO2. The integer logical units that are associated with these files are assigned by the block data statement located in BLKDAT.FOR. These logical units are passed throughout the program by the named common block statement in file IOUNIT.

All output files are deleted at the start of the program, as may be seen from looking at files MAIN.FOR and FILEOP.FOR. Thus, it is important to append any breakpoint information contained in X.SOUT to X.INN, as appropriate, *before* the next execution of the program, lest that which was stored in X.SOUT be overwritten and lost.

The second kind of data file involves the database of constituent media. These data files serve as input to subroutines, i.e., DIELxx, which calculate the constituent dielectric functions. Each data file is associated with a distinct constituent medium. Usually, the data file contains a discrete profile of the complex dielectric function and/or the complex refractive index as a function of energy. Naturally, the filenames must match that assumed

by the subroutines that read them. Here, the filenames are rather suggestive and straightforward, e.g., W.SI for crystalline silicon, W.SIA for amorphous silicon, W.SI3_N4 for noncrystalline Si_3N_4 , W.GA_AS for crystalline gallium arsenide, etc.

4.1.2 Allocation of Array or Work Space

In general, the allocation size of the arrays used in the program may be determined or estimated from a set of eight constants. These constants are assigned their numerical values prior to compilation by parameter statements located in file DEFNIT, see section 6.1.2. Consequently, if any changes are made to these assignments, it is usually necessary to recompile and relink most (if not all) of the subroutines in order to incorporate the said changes into the running program. The following list includes the eight basic constants.

nsampl, the maximum number of samples allowed for analysis, where the sample involves some finite number of films/layers atop a substrate.

nfilms, the maximum number of films/layers allowed atop the substrate of any given sample.

nparms, the maximum number of distinct parameters allowed per mixture or effective medium.

nlmnts, the maximum number of distinct constituent media (ϵ_j) allowed during analysis.

nbient, the maximum number of distinct ambients allowed atop the layers/substrate of any sample.

nwaves, the maximum number of distinct classical optical frequencies or wavelengths in vacuum of light incident on any sample.

nanglx, the maximum number of angles of incidence allowed per classical optical frequency of light incident on any sample.

nrpeat, the maximum number of repeats of an experiment run, where an experiment run involves taking measurements of (Δ, ψ) for a range of incident angles and energies on the same (ambient/sample) configuration.

In some cases, the array allocations are overestimated. The algorithms that estimate the array allocations from these eight constants assume a worst-case scenario involving the

largest size possible being calculated. This occurs especially when sizing arrays for the Jacobian. Here, it is convenient to assign some upper limit to these arrays. This is the purpose of the constant named `nnjaaa`. It is located in file `ARRAYS`, see section 6.1.7. A few internal check-tests are provided to help ensure that indices remain within bounds of the dimensions of these arrays.

4.1.3 Library Software

During the course of calculation of the least-squares fit, it is sometimes necessary to estimate the sensitivity of the model parameters. As discussed earlier in section 3.2, e.g., eq (22), it is necessary to calculate the inverse of a square matrix, i.e., the matrix formed by the product of the Jacobian and its transpose. This may be evaluated by using subroutines from the LINPACK library of mathematical software [15]. Reference calls to such subroutines may be found in subroutine `CORLAT`, see section 6.2.21.

4.2 Input Data Requirements

As mentioned previously in section 4.1.1, the input data file `X.DAT` contains: the model parameters, the characterization of the layered structure of the samples, and the measurement data of ellipsometric angles. Also, the input file contains information regarding the locations of the database files of point functions that are used in calculating the dielectric functions of the distinct constituent media. Here, all of the database files reside in the same directory.

The following subsections develop a line-by-line construction of file `X.DAT`. As mentioned above, the input data may be partitioned into subsets. Each subsection discusses one subset, and the subsets are presented in the order that they are expected to occur in the input file. Because each subset of data requires its own input format, each format is demonstrated with a worked example. For convenience, an example of a completed input file is presented in the last subsection, section 4.2.9.

The main program uses subroutine `INPDAT` to read all of the data in file `X.DAT`, see section 6.2.3. These data are stored in the arrays of named common areas; `FILMMM` and `XPRMNT`, see sections 6.1.3 and 6.1.4, respectively.

Note: The examples presented in this document are for the expressed single purpose of communicating the utility of the software package and are *not* to be construed as an endorsement of the *best* models or numerical values that may be assigned to the optical properties of the media at particular optical frequencies.

4.2.1 Database Information

Regarding the database of point functions that are used in evaluating dielectric functions of constituent media, as mentioned earlier in sections 2.1, 2.2, and 4.1.2, all these files are assumed to reside in the same directory. Further, since the complete specification of a file is of the form:

disk:[directory]filename.extension;version

when no defaults are assumed, it is convenient to let the database files have similar filenames, i.e., W, but have distinct extensions to identify distinct constituent media. Consequently, the first line of data in X.DAT is a character string which allows one to complete the specification of these files. Since the extension refers to a specific medium, the first line in X.DAT may contain everything *but* the extension. Incidentally, the file specification is completed by appending a character string of the appropriate extension that is stored in the subroutine that calculates the dielectric function of the constituent medium, i.e., DIELxx, where xx is a two-digit integer. An example of the format may be something like the following:

drb1:[data_bases]w.

where 'drb1' refers to the name of the disk or mass-storage device, 'data_bases' refers to the name of the directory, and 'w.' refers to the filename of the database files, i.e., including the final period and no extension.

4.2.2 Layer Thicknesses

The next set of data involves listing the distinct thicknesses of the layers that form the layered structure of the samples. The unit measure of thickness is nanometers.

As mentioned earlier in section 3, the numerical values assigned to these parameters may be selected to undergo variation (vary) or remain fixed (frozen) during the course of the

analysis or calculations. An integer switch (froz/vary) is provided for each model parameter, i.e., refractive index or extinction coefficient. If the switch is set equal to 0, the numerical value is frozen. If the switch is set equal to 1 upon input, the numerical value may undergo variation. The switches remain unchanged during the course of calculation.

An uncertainty value is also required for each model parameter. The magnitude of this uncertainty may serve either of two purposes. If the numerical value of the parameter undergoes variation, then the uncertainty value sets the maximum stepsize allowed for changing the numerical value of the parameter between consecutive iterations of the calculation. If the numerical value of the parameter is selected to remain frozen, then the uncertainty value is used during the sensitivity analysis calculation to estimate the uncertainty values of other 'vary' model parameters. This is discussed further in section 3.2.

To demonstrate the necessary format, it is convenient to consider an example of a sample that involves two layers atop a substrate of silicon, where one layer is atop the other layer. Let the layer adjacent to the ambient region be a thermally grown oxide. Let the layer adjacent to the substrate region be a thin transition region that involves some mixture of thermally grown oxide and crystalline silicon. The layered structure may then be expressed by the ordered form:

(ambient / oxide / oxide + silicon / silicon substrate).

Suppose further that the top layer of oxide is 100 nm thick, that the transition region is 2 nm thick, and that a reasonable initial estimate of the uncertainty is subjectively chosen to be 2 nm. Lastly, let only the transition region thickness be subject to optimization. This construct would require four lines of input data. An example of the format would be as the following:

```
-----
2          ! mfilmz ~ thicknesses /(i,z,zu,ivary)
1    100.0    2.0    0    !    i,z,zu,ivary ~ top layer, SiO2
2         2.0    2.0    1    !    i,z,zu,ivary ~ bottom layer, SiO2+Si
```

Note that the tabulation would include distinct thicknesses from all samples; thus any ordering among the thicknesses is not necessarily important here. Again, this format does not mention any sample or any ordering of layers; thus these thicknesses are not yet associated with any particular sample. The ordering of layers for a sample is presented later in section 4.2.7.

Also, note the initial line of connected hyphens; it is included. The intent here is to ease the readability of the input file. For convenience, a line of connected hyphens will be assumed to precede each format presented in the remaining subsections of 4.2.

Since the program uses READ statements to fetch its data from files, it is convenient to use a notation that is a suggestive adaptation of the argument list of a READ statement in FORTRAN. This notation was presented previously in [3]. Following this same convention for specifying input formats, the input format for thicknesses may be expressed by the form:

$$m_z / (i, z_i, \delta z_i, v_i)$$

where:

m_z is the number of distinct thicknesses that contribute to the layered structure of the samples;

i is an integer that indexes the line entries consecutively in unit increments, i.e., ($i = 1, 2, 3, \dots, m_z$);

z_i is the thickness of a layer measured in nanometers;

δz_i is the uncertainty that is assigned to the numerical value of z_i ; and

v_i is the integer (froz/vary) switch with value 0 or 1, respectively.

The forward slash mark '/' delimits the first line of input data. The parentheses bound items that ought to appear on each subsequent line of data until the implied DO-loop has been satisfied. Such notation has been convenient in conveying the complicated formats that are required for the input entries as well as the associated data structures. This notation is assumed throughout the remainder of the document unless inferred otherwise from context.

Incidentally, if ($m_z = 0$), this is the only line of information that ought to be entered for this set of data, i.e., apart from the short line of connected hyphens.

4.2.3 Supplementary Parameters (Integer)

Regarding the ability of the program to incorporate complicated models, it is sometimes important to be able to pass parameters to subroutines that calculate the dielectric functions of the constituents and mixtures. Such parameters may serve as integer switches for decision processes or serve as floating-point variables that may be subjected to optimization. The manner in which these parameters are discerned and passed among the subroutines may be readily seen by considering the subroutine named DIEFCN, see section 6.4.1. Although the structure for passing, referring, and interpreting the supplementary parameters is rather limited, it does provide some measure of convenience for the user in adapting or incorporating his/her own models. The input format for integer supplementary parameters is of the form:

$$m_I / (i, p_i)$$

where:

m_I is the number of distinct integer supplementary parameters;

i is an integer that indexes the line entries of data consecutively in unit increments, i.e., ($i = 1, 2, 3, \dots, m_I$); and

p_i is the integer supplementary parameter.

Since integer parameters are not subjected to optimization here, no uncertainties are included regarding their numerical value. This tabulation includes all integer supplementary parameters that may be associated with any of the samples or mixtures.

Since the integer supplementary parameters are used so infrequently, it is often the case that ($m_I = 0$). Then, an example of the format would be of the form:

```
-----  
0                               ! mipars / (i,ip)
```

4.2.4 Supplementary Parameters (Floating-Point)

As mentioned above, the program provides the capability to input floating-point supplementary parameters to aid in modeling the optical behavior of the constituents and/or

mixtures. As may be seen from eq (7), these parameters may be subjected to optimization. The input format is of the form:

$$m_R / (i, p_i, \delta p_i, v_i)$$

where:

m_R is the number of distinct floating-point supplementary parameters;

i is an integer that indexes the line entries of data consecutively in unit increments, i.e., ($i = 1, 2, 3, \dots, m_R$);

p_i is the floating-point supplementary parameter;

δp_i is the uncertainty that is assigned to the numerical value of p_i ; and

v_i is the integer (froz/vary) switch with value of either 0 or 1, respectively.

Since the floating-point supplementary parameters are used so infrequently, it is often the case that ($m_R=0$). Then, an example of the format would be of the form:

```
-----
0 ! mrpars / (i,rp,up,ivary)
```

4.2.5 Effective Media or Mixtures

For each effective medium that contributes toward the construction of the layered structure of the sample, as well as the ambient regions, one must specify the constituents and their volume fractions. If any constituent medium requires supplementary parameters, it is convenient to include this information as well. Further, it is convenient to group such information individually. Regarding the organization of these data for the effective media, the general format is given by the following form:

m_{media}

$m_{f,1}$	$\dots$				
$\vdots$					
$m_{f,j-1}$	$\dots$				
	$\vdots$				
$m_{f,j}$	$m_{I,j}$	$m_{R,j}$			
	1	$\tilde{e}_1$	f_1	δf_1	v_1
	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
	i_f	$\tilde{e}_i$	f_i	δf_i	v_i
	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
	$m_{f,j}$	$\tilde{e}_{m_{f,j}}$	$f_{m_{f,j}}$	$\delta f_{m_{f,j}}$	$v_{m_{f,j}}$
	1	$\tilde{p}_{I,1}$			
	$\vdots$	$\vdots$			
	i_I	$\tilde{p}_{I,i}$			
	$\vdots$	$\vdots$			
	$m_{I,j}$	$\tilde{p}_{I,m_{I,j}}$			
	1	$\tilde{p}_{R,1}$			
	$\vdots$	$\vdots$			
	i_R	$\tilde{p}_{R,i}$			
	$\vdots$	$\vdots$			
	$m_{R,j}$	$\tilde{p}_{R,m_{R,j}}$			
$m_{f,j+1}$	$\dots$				
$\vdots$					
$m_{f,m_{\text{media}}}$	$\dots$				
	$\vdots$				

where

m_{media} is the number of distinct effective media. From sections 4.1.2 and 6.1.2,
 $(2 \leq m_{\text{media}} \leq \text{nsampl} * (\text{nfilms} + 2))$.

j is an integer that indexes the distinct effective media, i.e., $(j = 1, 2, \dots, m_{\text{media}})$.

$m_{f,j}$ is the number of distinct constituent media (or volume fractions) that are associated with the j^{th} effective medium. From section 4.1.2, $(1 \leq m_{f,j} \leq \text{nlmnts})$.

$m_{I,j}$ is the number of integer supplementary parameters that are associated with the j^{th} effective medium.

$m_{R,j}$ is the number of floating-point supplementary parameters that are associated with the j^{th} effective medium.

i_f is an integer that locally indexes the distinct constituent media (or volume fractions) of the j^{th} effective medium, i.e., $(i_f = 1, 2, \dots, m_{f,j})$. For convenience and readability, the subscript j on i is suppressed here, as well as in the following set of entries.

$\tilde{e}_i$ is an integer index label of the appropriate constituent medium that is associated with the i_f^{th} constituent medium of the j^{th} effective medium. From section 4.1.2, $(1 \leq \tilde{e}_i \leq \text{nlmnts})$.

f_i is the volume fraction of the i_f^{th} constituent medium of the j^{th} effective medium.

δf_i is the uncertainty that is assigned to the numerical value of f_i .

v_i is the integer (froz/vary) switch for f_i with value 0 or 1, respectively.

i_I is an integer that locally indexes the integer supplementary parameters that are associated with the j^{th} effective medium, i.e., $(i_I = 1, 2, \dots, m_{I,j})$.

$\tilde{p}_{I,i}$ is the integer index label of the appropriate integer supplementary parameter that is associated with the i_I^{th} integer supplementary parameter of the j^{th} effective medium, i.e., $(1 \leq \tilde{p}_{I,i} \leq m_I)$, where m_I was presented earlier in section 4.2.3.

i_R is an integer that locally indexes the floating-point supplementary parameters that are associated with the j^{th} effective medium, i.e., $(i_R = 1, 2, \dots, m_{R,j})$.

$\tilde{p}_{R,i}$ is the integer index label of the appropriate floating-point supplementary parameter that is associated with the i_R^{th} floating-point supplementary parameter of the j^{th} effective medium, i.e., $(1 \leq \tilde{p}_{R,i} \leq m_R)$, where m_R was presented earlier in section 4.2.4.

Again, regarding the above entries that are capped with a tilde, it is important to note that these entries refer to index labels local to the appropriate subset of data, i.e., constituent media and supplementary parameters from sections 4.2.1, 4.2.3, and 4.2.4.

To demonstrate this format, consider again the example that was presented in section 4.2.2 regarding thicknesses. The layered structure involved the following ordered form:

(ambient / oxide / oxide + silicon / silicon substrate).

This structure involves four distinct effective media, i.e., one for each distinct spatial region. Letting the ambient be air, one need only consider three distinct constituent media, i.e., air, oxide, and silicon.

In section 6.5, one may locate the set of distinct constituent media that is of interest here, and then go on to identify the names of the subroutines which are used to calculate the dielectric functions, i.e., DIELxx, where xx refers to some two-digit number. Here, the index label that is associated with a distinct constituent medium is that integer which is derived from the last two characters of the subroutine name, i.e., xx. The constituent media index labels for air, silicon, and oxide are found to be 2, 3, and 5, respectively. Further, let the transition region be half oxide and half silicon. The format for this example could then be as the following:

```

-----
4                               ! mixtures ~ number of effective media
1  0  0                        !   mlmnt,mipar,mrpar          #1
    1  2  1.0  0.0  0          !       j,lmnt,frac,ufrac,ivary ~ air
1  0  0                        !   mlmnt,mipar,mrpar          #2
    1  3  1.0  0.0  0          !       j,lmnt,frac,ufrac,ivary ~ Si
1  0  0                        !   mlmnt,mipar,mrpar          #3
    1  5  1.0  0.0  0          !       j,lmnt,frac,ufrac,ivary ~ SiO2
2  0  0                        !   mlmnt,mipar,mrpar          #4
    1  3  0.5  0.02  1         !       j,lmnt,frac,ufrac,ivary ~ Si
    2  5  0.5  0.02  1         !       j,lmnt,frac,ufrac,ivary ~ SiO2

```

The uncertainties of the volume fractions of the transition region have been subjectively set at 0.02, and the volume fractions of the transition region have been selected to undergo optimization. Again, because the volume fractions must sum to one, the number of volume fractions that may be selected to undergo variation may be set equal to 0, 2, or more than 2. Although the line entries of the constituent media are not necessarily ordered, the constituent media must be distinct. This is check-tested; a violation stops the program. Regarding the comments that are appended onto each line of data, the word 'lmnt' is a mnemonic for *elements* or constituents. Lastly, since the format simply tabulates distinct effective media, ordering of the distinct effective media is not important here.

4.2.6 Ambients and External Parameters

The ambient region refers to that spatial region that lies external to the layered structure of the sample, i.e., the (layers/substrate) system. Sometimes, it is necessary to analyze ellipsometric measurements involving a number of distinct samples and ambients. In the Table of Contents, it may be seen that the database contains at least two distinct constituent media which are often used as ambients, i.e., vacuum and air.

Of course, the database may be enlarged to include nearly any number of lossless, isotropic, and homogeneous media. Enlarging the database is rather straightforward, because the user need only follow the conventions that are assumed by subroutine DIELMN, see section 6.4.4.

Because the analysis of a sample may involve more than one ambient, it is convenient to construct an indexed listing of effective media that are used as ambients. Further, in the event that a distinct (ambient/sample) system depends upon some independent or *external* parameter, e.g., an externally applied perturbation or stress field, this information may be included in the indexed listing as well. The indexed listing defines an ambient as being that composite entity which associates a distinct effective medium and two distinct sets of supplementary parameters that characterize the applied perturbation.

The indexed listing of the ambients simply provides another opportunity for assigning supplementary parameters to the effective or constituent media of the system configuration. The general format is given by the following form:

m_{ambients}

	1	...		
	$\vdots$			
	$(j-1)$	...		
	$\vdots$			
	j	$\tilde{e}_j$	$m_{I,j}$	$m_{R,j}$
		1	$\tilde{p}_{I,1}$	
		$\vdots$	$\vdots$	
		i_I	$\tilde{p}_{I,i}$	
		$\vdots$	$\vdots$	
		$m_{I,j}$	$\tilde{p}_{I,m_{I,j}}$	
		1	$\tilde{p}_{R,1}$	
		$\vdots$	$\vdots$	
		i_R	$\tilde{p}_{R,i}$	
		$\vdots$	$\vdots$	
		$m_{R,j}$	$\tilde{p}_{R,m_{R,j}}$	
	$(j+1)$	...		
	$\vdots$			
m_{ambients}		...		
		$\vdots$		

where

m_{ambients} is the number of distinct ambients which involves associating distinct effective media with subsets of supplementary parameters for all configurations of the (ambient/sample) system. From sections 4.1.2 and 6.1.2, $(1 \leq m_{\text{ambients}} \leq \text{nbient})$.

j is an integer that indexes the distinct ambients, i.e., $(j = 1, 2, \dots, m_{\text{ambients}})$.

$\tilde{e}_j$ is an integer index label of the appropriate effective (*not* constituent) medium that is associated with the j^{th} ambient. From section 4.2.5, $(1 \leq \tilde{e}_j \leq m_{\text{media}})$.

$m_{I,j}$ is the number of integer supplementary parameters that are associated with the j^{th} ambient.

$m_{R,j}$ is the number of floating-point supplementary parameters that are associated with the j^{th} ambient.

i_I is an integer that locally indexes the integer supplementary parameters that are associated with the j^{th} ambient, i.e., ($i_I = 1, 2, \dots, m_{I,j}$). For convenience and readability, the subscript j on i is suppressed here, as well as in the following set of entries.

$\tilde{p}_{I,i}$ is the integer index label of the appropriate integer supplementary parameter that is associated with the i_I^{th} integer supplementary parameter of the j^{th} ambient, i.e., ($1 \leq \tilde{p}_{I,i} \leq m_I$), where m_I was presented earlier in section 4.2.3.

i_R is an integer that locally indexes the floating-point supplementary parameters that are associated with the j^{th} ambient, i.e., ($i_R = 1, 2, \dots, m_{R,j}$).

$\tilde{p}_{R,i}$ is the integer index label of the appropriate floating-point supplementary parameter that is associated with the i_R^{th} floating-point supplementary parameter of the j^{th} ambient, i.e., ($1 \leq \tilde{p}_{R,i} \leq m_R$), where m_R was presented earlier in section 4.2.4.

Again, regarding the above entries that are capped with a tilde, it is important to note that these entries refer to index labels local to the appropriate subset of data, i.e., supplementary parameters and effective media presented in sections 4.2.3, 4.2.4, and 4.2.5.

To demonstrate this format, it is convenient to build upon the development of the previous example. The format for the ambient configurations could then be as the following:

```
-----
1                               ! mbient " number of ambients
  1  1  0  0                   !   j,imix,mipar,mrpar           " air
```

because no supplementary parameters have been used thus far; the worked examples in sections 4.2.3 and 4.2.4 assumed that ($m_I = m_R = 0$).

4.2.7 Sample Characterization or Construction

Now that the basic model parameters have been presented, it is possible to discuss the method of constructing a sample by characterizing each region of its layered structure in terms of the basic parameters presented heretofore. From section 4.1.2, the program is able to analyze a number of distinct samples collectively. Here, the samples become indexed according to the order in which they are entered for characterization in the input file. Furthermore, this ordering of samples will also govern how the measurement data are to be entered in the file; such is discussed later in the next subsection.

First, it is important to discuss the meaning of the word *sample*. A sample is defined as being that material structure of the (layers/substrate) system that is subjected to ellipsometric measurement. The business of characterizing a sample refers to that procedure of index-labeling which associates the distinct spatial regions of the (layers/substrate) system with the appropriate sets of model parameters, so that the direct or forward problem may be completely defined, i.e., apart from specifying the ambient. Since measurements on a sample may involve more than one ambient, the business of associating samples and ambients is deferred until the next subsection. Here, the samples are constructed or assembled in a layer-by-layer fashion. For each spatial region, one must specify an effective medium, and if the region is a layer, one must also specify a thickness.

Recall, the inverse problem is formulated as a least-squares problem. This involves a series of linear algebra problems. Consequently, the matrices associated with individual samples may be combined so that several samples may be analyzed together. Here, the program is said to have a multiple-sample capability. The maximum number of samples that may be analyzed together is set by the parameter `nsamp1`, as mentioned in section 4.1.2.

Each previous subsection presented a format for inputting parameters. Each model parameter has a distinct index label; each line entry following the first line is usually indexed. Here, those index labels are used for specifying the configuration of the (layers/substrate) system. The sample is characterized by an ordered set of integers that point into those arrays which store the numerical values of the parameters.

The general format for specifying the layered structure of the samples is of the following form:

$$\begin{array}{ccccc}
m_{\text{samples}} & & & & \\
& m_{z,1} & & & \\
& \vdots & & & \\
& m_{z,j} & & & \\
& & 1 & \tilde{e}_1 & \tilde{z}_1 \\
& & \vdots & \vdots & \vdots \\
& & i & \tilde{e}_i & \tilde{z}_i \\
& & \vdots & \vdots & \vdots \\
& & m_{z,j} & \tilde{e}_{m_{z,j}} & \tilde{z}_{m_{z,j}} \\
& & (m_{z,j}+1) & \tilde{e}_{\text{substrate},j} & \\
& m_{z,(j+1)} & & & \\
& \vdots & & & \\
m_{z,m_{\text{samples}}} & & & & \\
& \vdots & & &
\end{array}$$

where

m_{samples} is the number of distinct material samples that are subjected to ellipsometric measurement. From section 4.1.2, $(1 \leq m_{\text{samples}} \leq \text{nsampl})$.

j is an integer that indexes the distinct samples, i.e., $(j = 1, 2, \dots, m_{\text{samples}})$.

$m_{z,j}$ is the number of layers that lie atop the substrate of the j^{th} sample.

From section 4.1.2, $(0 \leq m_{z,j} \leq \text{nfilms})$.

i is an integer that locally indexes the distinct layers of the j^{th} sample, i.e., $(i = 1, 2, \dots, m_{z,j})$. The layer adjacent to the ambient is indexed 1; the layer adjacent to the substrate is indexed $m_{z,j}$. For convenience and readability, the subscript j on i is suppressed here, as well as in the following set of entries.

$\tilde{e}_i$ is the integer index label of the appropriate effective medium that is associated with the i^{th} layer of the j^{th} sample. From section 4.2.5, $(1 \leq \tilde{e}_i \leq m_{\text{media}})$.

$\tilde{z}_i$ is the integer index label of the appropriate thickness that is associated with the i^{th} layer of the j^{th} sample. From section 4.2.2, $(1 \leq \tilde{z}_i \leq m_z)$.

Again, regarding the above entries that are capped with a tilde, it is important to note that these entries refer to index labels local to the appropriate subset of data, i.e., effective media and thicknesses presented in sections 4.2.5 and 4.2.2, respectively.

To demonstrate this format, it is convenient to build upon the development of the previous example. Again, the sample involved the form: (oxide / oxide + silicon / silicon substrate). The format for this sample configuration would then be as the following:

```

-----
1          ! msampl  ~ number of samples analyzed
2          !      mfilm ~ number of layers on sample #1
      1  3  1          !      j,imix,iz  ~ SiO2    , top layer
      2  4  2          !      j,imix,iz  ~ SiO2+Si, transition region
      3  2          !      j,imix      ~ Si      , substrate

```

No mention is made regarding the ambient; this is discussed in the next subsection.

4.2.8 Measurement Data (Δ, ψ)

The measurement data of ellipsometric angles are organized in the same fashion as was presented in the previous subsection, i.e., sample by sample. Regarding measurements, both the sample and ambient must be specified. To characterize the (ambient/sample) system, a similar scheme of index labels is assumed again.

For convenience, the integers are ordered in a format compatible with the collection algorithm of the laboratory instrumentation. The ellipsometric measurement data are ordered into a data structure that follows the FORTRAN indexing convention for multiply-indexed arrays. That data structure is of the following form:

(*angles & wavelengths, repeats, ambients, samples*)

where:

samples indexes the set of distinct samples that were subjected to ellipsometric measurement;

ambients indexes the set of distinct ambients used during measurement involving a given sample;

repeats indexes the sets of distinct repeats of multiple-angle of incidence and multiple-optical frequency measurements performed on a system involving a given ambient and sample; and

angles & wavelengths indexes the set of distinct angles of incidence and optical frequencies (or wavelengths) used during measurement on a system of given repeat index, ambient, and sample.

This form suggests that the measurement data (Δ, ψ) are grouped and ordered according to the following structure. The measurement data are grouped sample by sample. For each sample, they are grouped ambient by ambient. For each ambient, they are grouped by their repeat index label. For each repeat index, they are indexed by the source variables, i.e., the angle of incidence and the optical frequency (or wavelength in vacuum or corresponding photon energy) of the light. Ordering among the incident angles or among the optical frequencies is not important, i.e., apart from that associated with the input format. Hence, the forward problem becomes completely defined. The *repeats* simply partition the measurement data, e.g., distinguishing measurement data collected on different days.

To implement the above organization and thereby characterize the (ambient/sample) system, the program reads a tabulated set of integers line by line. Since the program assumes that data are entered sample by sample, one need only consider the data for one sample, e.g., sample s . The total set of input data of all samples is constructed simply by concatenating the individual data sets of each sample. Now, consider the data that are associated with sample s . The first line of data is the number of ambients, m_{as} .

Let a_s index the set of distinct ambients on sample s . Let $\tilde{a}_s$ be the index label of the appropriate ambient that is associated with the a_s^{th} ambient on sample s . Let m_{ras} be the number of sets of repeat measurements of (Δ, ψ) involving the a_s^{th} ambient on sample s . Let r_{as} index these sets of repeat measurements. Heading the set of data associated with the a_s^{th} ambient would be a line that contains two integers, m_{ras} and $\tilde{a}_s$.

The ordering infers that r_{as} is sequenced through its range *before* the indexing of a_s is stepped; i.e., repeated sets of measurements on a sample are collected together before one considers changing the ambient.

Since the (*repeat, ambient, sample*) structure is an ordered form, the structure is completely specified by the aforementioned indices. Next, consider the data of the r_{as}^{th} repeat set. Heading this set of data would be a line that contains one integer, the number of measurements of (Δ, ψ) . It is denoted by $m_{\lambda\phi, ras}$. For convenience, it is not necessary to include the indexing label r_{as} on the same line.

This is followed by the measurement data of ellipsometric angles. They are entered into the data file line by line. Each set of measurements involves two lines of data, one being for the source variables (λ, ϕ) and measured ellipsometric angles (Δ, ψ) , and the other being for the associated uncertainties. The format is of the following form:

$$m_{\lambda\phi, ras} / (i, \lambda_i, \phi_i, \Delta_i, \psi_i / \delta\lambda_i, \delta\phi_i, \delta\Delta_i, \delta\psi_i)_{ras}$$

where:

$m_{\lambda\phi, ras}$ is the total number of measurements of ellipsometric angles (Δ, ψ) involving multiple angles of incidence and multiple optical frequencies that involve the r_{as}^{th} repeat set of measurements, i.e., $(r_{as} = 1, 2, \dots, m_{ras})$, and the a_s^{th} ambient of sample s , i.e., $(a_s = 1, 2, \dots, m_{as})$. From sections 4.1.2, 6.1.2, and 6.2.3, $(1 \leq m_{\lambda\phi, ras} \leq \text{nwaves} * \text{nanglx} \leq \text{nexpts})$.

i is an integer that locally indexes the multiple-angle of incidence and multiple-optical frequency measurement data consecutively with unit increments, i.e., $(i = 1, 2, \dots, m_{\lambda\phi, ras})$.

λ_i is a floating-point source parameter that may be of either sign depending upon how one chooses to characterize the optical frequency of light. When the value is negative, the unit of measure is nanometers. When the value is positive, the unit of measure is electron-volts. The program check-tests for either $(-1240 \leq \lambda_i \leq -200)$ or $(1.0 \leq \lambda_i \leq 6.0)$.

$\delta\lambda_i$ is the uncertainty that is assigned to the numerical value of λ_i .

ϕ_i is the angle of incidence measured in degrees, where a value of zero relates to that of normal incidence, i.e., $(0 \leq \phi_i \leq 90)$.

$\delta\phi_i$ is the uncertainty that is assigned to the numerical value of ϕ_i .

Δ_i is an ellipsometric angle measured in degrees, i.e., $(0 \leq \Delta_i < 360)$, assuming the Nebraska convention, i.e., $R_{p,H}$ from section 2.3 of [3].

$\delta\Delta_i$ is the uncertainty that is assigned to the numerical value of Δ_i .

ψ_i is an ellipsometric angle measured in degrees, i.e., $(0 \leq \psi_i \leq 90)$.

$\delta\psi_i$ is the uncertainty that is assigned to the numerical value of ψ_i .

Within any set of $m_{\lambda\phi,ras}$ measurement data, ordering of optical frequencies or angles of incidence is not important. Thus, regarding sample s , the general format is given by the following form:

$$\begin{array}{cccccc}
 m_{as} & & & & & \\
 & \vdots & & & & \\
 & m_{ras} & \tilde{a}_s & & & \\
 & & \vdots & & & \\
 & & m_{\lambda\phi,ras} & & & \\
 & & & \vdots & & \\
 & & i & \lambda_i & \phi_i & \Delta_i & \psi_i \\
 & & & \delta\lambda_i & \delta\phi_i & \delta\Delta_i & \delta\psi_i \\
 & & & \vdots & & &
 \end{array}$$

Again, to construct the final set of data for all of the samples, one simply concatenates the data for each individual sample, i.e., without any intervening lines of demarcation.

To demonstrate this format, let the measurements be those found by solving the forward problem for the (ambient/sample) configuration that was developed in the previous examples. Hence, these measurements would be *exact*. Let the measurements involve a grid of optical frequencies, e.g., where the associated photon energies are between 1.5 to 6.0 eV in steps of 0.5 eV, for one angle of incidence, e.g., 70 deg. Let $\delta\lambda$, $\delta\phi$, $\delta\Delta$, and $\delta\psi$ be given by 0.1, 0.01, 0.01, and 0.01 deg, respectively. Although these uncertainties depend on the instrumentation, the values are chosen subjectively for convenience. The format could then be as the following:

```

-----
1          ! mbien " number of ambients on sample #1
1 1        ! mrpeat,imbien
10         ! mexpt " number of measurements
1 1.50000E+00 7.00000E+01 8.04309E+01 3.08875E+01 (i,E,a, d,p)
1.00000E-01 1.00000E-02 1.00000E-02 1.00000E-02 (uncertainty)
2 2.00000E+00 7.00000E+01 7.97129E+01 4.31275E+01 (i,E,a, d,p)
1.00000E-01 1.00000E-02 1.00000E-02 1.00000E-02 (uncertainty)
3 2.50000E+00 7.00000E+01 1.02227E+02 6.93018E+01 (i,E,a, d,p)
1.00000E-01 1.00000E-02 1.00000E-02 1.00000E-02 (uncertainty)
4 3.00000E+00 7.00000E+01 2.50415E+02 6.09989E+01 (i,E,a, d,p)
1.00000E-01 1.00000E-02 1.00000E-02 1.00000E-02 (uncertainty)
5 3.50000E+00 7.00000E+01 2.62427E+02 4.00376E+01 (i,E,a, d,p)
1.00000E-01 1.00000E-02 1.00000E-02 1.00000E-02 (uncertainty)
6 4.00000E+00 7.00000E+01 2.47313E+02 3.31054E+01 (i,E,a, d,p)
1.00000E-01 1.00000E-02 1.00000E-02 1.00000E-02 (uncertainty)
7 4.50000E+00 7.00000E+01 1.92800E+02 3.34557E+01 (i,E,a, d,p)
1.00000E-01 1.00000E-02 1.00000E-02 1.00000E-02 (uncertainty)
8 5.00000E+00 7.00000E+01 1.24499E+02 3.21867E+01 (i,E,a, d,p)
1.00000E-01 1.00000E-02 1.00000E-02 1.00000E-02 (uncertainty)
9 5.50000E+00 7.00000E+01 8.77637E+01 3.66717E+01 (i,E,a, d,p)
1.00000E-01 1.00000E-02 1.00000E-02 1.00000E-02 (uncertainty)
10 6.00000E+00 7.00000E+01 7.10687E+01 4.18238E+01 (i,E,a, d,p)
1.00000E-01 1.00000E-02 1.00000E-02 1.00000E-02 (uncertainty)

```

Incidentally, these data are retained in arrays that are located in the named common area, `exprmt`, see section 6.1.4.

4.2.9 Combining

In general, the input data are composed of two kinds of information, those which define the system model and associated measurements, and those which define the options for processing these data. Thus far, only the first kind has been presented, and they are contained in the input file `X.DAT`. The input data file is constructed by simply combining the formats in the order that they were presented. In general, no intervening blank lines are allowed. Again, those lines of connected hyphens are merely conveniences; the intent is that of easing the readability of the input file.

Combining the examples of the formats presented thus far, and indexing the lines for convenience, i.e., the input data file would *not* actually contain such indexing, the input data file `X.DAT` would become:


```

1 drb1:[data_bases]w.
2 -----
3 2 ! mfilmz " thicknesses /(i,z,zu,ivary)
4 1 100.0 2.0 0 ! i,z,zu,ivary " top layer, SiO2
5 2 2.0 2.0 1 ! i,z,zu,ivary " bottom layer, SiO2+Si
6 -----
7 0 ! mipars / (i,ip)
8 -----
9 0 ! mrpars / (i,rp,up,ivary)
10 -----
11 4 ! mixtures " number of effective media
12 1 0 0 ! mlmnt,mipar,mrpar #1
13 1 2 1.0 0.0 0 ! j,lmnt,frac,ufrac,ivary " air
14 1 0 0 ! mlmnt,mipar,mrpar #2
15 1 3 1.0 0.0 0 ! j,lmnt,frac,ufrac,ivary " Si
16 1 0 0 ! mlmnt,mipar,mrpar #3
17 1 5 1.0 0.0 0 ! j,lmnt,frac,ufrac,ivary " SiO2
18 2 0 0 ! mlmnt,mipar,mrpar #4
19 1 3 0.5 0.02 1 ! j,lmnt,frac,ufrac,ivary " Si
20 2 5 0.5 0.02 1 ! j,lmnt,frac,ufrac,ivary " SiO2
21 -----
22 1 ! mbient " number of ambients
23 1 1 0 0 ! j,imix,mipar,mrpar " air
24 -----
25 1 ! msampl " number of samples analyzed
26 2 ! mfilm " number of layers on sample #1
27 1 3 1 ! j,imix,iz " SiO2 , top layer
28 2 4 2 ! j,imix,iz " SiO2+Si, transition region
29 3 2 ! j,imix " Si , substrate
30 -----
31 1 ! mbien " number of ambients on sample #1
32 1 1 ! mrpeat,mbien
33 10 ! mexpt " number of measurements
34 1 1.50000E+00 7.00000E+01 8.04309E+01 3.08875E+01 (i,E,a, d,p)
35 1.00000E-01 1.00000E-02 1.00000E-02 1.00000E-02 (uncertainty)
36 2 2.00000E+00 7.00000E+01 7.97129E+01 4.31275E+01 (i,E,a, d,p)
37 1.00000E-01 1.00000E-02 1.00000E-02 1.00000E-02 (uncertainty)
38 3 2.50000E+00 7.00000E+01 1.02227E+02 6.93018E+01 (i,E,a, d,p)
39 1.00000E-01 1.00000E-02 1.00000E-02 1.00000E-02 (uncertainty)
40 4 3.00000E+00 7.00000E+01 2.50415E+02 6.09989E+01 (i,E,a, d,p)
41 1.00000E-01 1.00000E-02 1.00000E-02 1.00000E-02 (uncertainty)
42 5 3.50000E+00 7.00000E+01 2.62427E+02 4.00376E+01 (i,E,a, d,p)
43 1.00000E-01 1.00000E-02 1.00000E-02 1.00000E-02 (uncertainty)
44 6 4.00000E+00 7.00000E+01 2.47313E+02 3.31054E+01 (i,E,a, d,p)
45 1.00000E-01 1.00000E-02 1.00000E-02 1.00000E-02 (uncertainty)
46 7 4.50000E+00 7.00000E+01 1.92800E+02 3.34557E+01 (i,E,a, d,p)
47 1.00000E-01 1.00000E-02 1.00000E-02 1.00000E-02 (uncertainty)
48 8 5.00000E+00 7.00000E+01 1.24499E+02 3.21867E+01 (i,E,a, d,p)
49 1.00000E-01 1.00000E-02 1.00000E-02 1.00000E-02 (uncertainty)
50 9 5.50000E+00 7.00000E+01 8.77637E+01 3.66717E+01 (i,E,a, d,p)
51 1.00000E-01 1.00000E-02 1.00000E-02 1.00000E-02 (uncertainty)
52 10 6.00000E+00 7.00000E+01 7.10687E+01 4.18238E+01 (i,E,a, d,p)

```

The example shows that three model parameters are selected for optimization; see lines 5, 19, and 20. These model parameters are associated with the transition region; see line 28. Hence, their numerical values will undergo variation if so requested from the command options in file X.INN. The command options are discussed in the next section.

Further, regarding model parameters selected for optimization, their uncertainty values were set to nonzero values. This condition is check-tested upon input; if violated, the user would be so notified of the zero values. Setting the uncertainty value to a nonzero value circumvents notification. The reason for the check-test is that the program uses the uncertainty value to limit the stepsize for updating the numerical value of the associated model parameter. With an allowed maximum stepsize of zero, the program would be unable to reduce the numerical value of the error expression, at least with respect to this model parameter. Being unable to justify further calculation, it would terminate. Such control is useful in other situations as well, e.g., limiting the calculation to a single evaluation of the residual or discerning relative contributions made to the uncertainty value of some 'vary' model parameter. This may be accomplished by assigning a sufficiently small number to the uncertainty value on input.

4.3 Command Options

As mentioned previously in section 4.1.1, the input data file X.INN contains the command options that are necessary for directing control of the software package. To direct the execution of the program, a menu-driven decision tree of command options is made available to the user. Incidentally, the program reads file X.DAT *before* reading file X.INN. Examples of X.INN files are shown in section 5.

The first level of the tree involves a menu of three options. One option is selected per execution of the program; the selection of that option is the first line of data in X.INN. After reading this line of input data, the program branches to the appropriate subroutine. After leaving this subroutine at level one, the main program stops. Hence, the main program does not loop back on itself to a condition where a request is made of the user to select another option at level one. This branching at level one is performed by the MAIN program, see section 6.2.1.

Before reading the first line of data in file X.INN, the MAIN program writes to the output file X.OUT the following menu of available options (at level one):

```
Enter:  option
        1, forward problems, plots, ...
        2, search      (vary)
        3, search grid (vary)
```

Where the options at level one include:

- 1, requests the program to perform one of several simple tasks, such as providing a set of tabulated output that is amenable for plotting or initiating a series of calculations of the direct or forward problem. No iterative calculations are considered, i.e., no minimizations or inversions of the ellipsometric equations. This is discussed further in section 4.3.1.
- 2, requests the program to invert the ellipsometric equations by performing a series of unconstrained optimization calculations. The variation of numerical values of selected model parameters is generally unbounded. This is presented in section 4.3.2.
- 3, requests the program to invert the ellipsometric equations by performing a grid scan over a selected set of model parameters. A series of constrained optimization calculations is initiated at each point of the grid of model parameters. This is discussed further in section 4.3.3.

These options provide the current range of utility of the program. Regarding the general nature of the options, it may be expected that option one is more useful towards the beginning of analysis with plots, while options two and three form the primary tools during analysis. Since the grid scans are constructed from a simple nesting of DO-loops, there may be redundant calculations over parts of the parameter space whenever the 'vary' model parameters are not common to every sample. These options are discussed further in the following subsections. Here, it is convenient to simply follow the decision tree of options.

4.3.1 Forward Problems, Plots, ...

Following the selection of option '1' at level one, the program calls subroutine SCATOS, thus entering level two, see section 6.2.4. This subroutine presents the user with another

set of options. The options specify the sets of source variables (λ, ϕ) that may be used in the model calculations. The menu of options at level two is:

```
Enter:  choice of incident (energies, angles)
        1,  measurement data,      x.dat
        2,  grid scan.
```

where the options involve:

- 1, requests the program to use as source variables only those sets of ordered pairs (λ, ϕ) that are specified in the input file X.DAT for the measurement data of (Δ, ψ) .
- 2, requests the program to use as source variables only those sets of ordered pairs (λ, ϕ) that lie on a two-dimensional grid that is specified later in a following prompt-request. The program prompts or requests information regarding the lower bound, the upper bound, and the stepsize for each dimension of the grid.

The above two options form a branch in the decision tree of options. The next step in the program involves specifying which field quantities are to be calculated and then written to the output file X.PLOT. Thus, another set of options is presented to the user, i.e., level three, but here the menu will depend upon which option is selected at level two. Hence, there are two alternative sets of options at level three. They are presented in succession.

After selecting option '1' at level two, the menu of options at level three is:

```
Enter:  choice of output suitable for:
        1,  input data,      x.dat,
        2,  plotting (Delta, psi),
        3,  plotting (Delta, psi) deviations,
            deviation = measurement - model.
        4,  plotting |g| ~ rms deviation, unscaled,
            on a 1D or 2D grid of model parameters.
```

where

- 1, requests the program to calculate (Δ, ψ) using (λ, ϕ) as supplied by the file X.DAT. The output is written to the plot file X.PLOT. The format is suitable for use in file X.DAT.
- 2, requests the program to calculate (Δ, ψ) using (λ, ϕ) as supplied by the file X.DAT.

The output is written to the plot file X.PLOT. The format is suitable for later graphics.

- 3, requests the program to calculate and tabulate the deviations between the measurement data and that calculated by the model. The deviations are ordered similar to that of the measurement data. The output is written to the plot file X.PLOT.
- 4, requests the program to initiate a grid scan of model parameters and evaluate the error expression $|g|$ for each point on the grid. For convenience, the grid may be either one or two dimensional; i.e., only one or two model parameters may undergo variation. It is then necessary to specify the domain of the grid. The format for specifying the grid of model parameters is presented later in section 4.3.3. But unlike that presented in section 4.3.3, there is no option regarding optimization here. The output is written to file X.PLOT.

After selecting option '2' at level two, the menu of options at level three is:

```
Enter:  choice of output suitable for:
        1,  dielectric function,  media,
        2,  (Delta, psi),          x.dat,
        3,  (Delta, psi),          plotting,
        4,  d/db,                  b'(z,f,p),
        5,  d/da,                  angle of incidence,
        6,  d/dE,                  energy.
```

where

- 1, requests the program to calculate the dielectric function for an effective medium that is specified in a later prompt-request from the program. The format is suitable for later graphics.
- 2, requests the program to calculate (Δ, ψ) for a grid of (λ, ϕ) . The format is suitable for use in file X.DAT.
- 3, requests the program to calculate (Δ, ψ) for a grid of (λ, ϕ) . The format is suitable for later graphics.
- 4, requests the program to calculate partial derivatives of (Δ, ψ) with respect to one of the model parameters, i.e., thickness, volume fraction, or supplementary parameter. Since volume fractions involve a linear constraint, the partial derivative with

respect to $\hat{f}_j$ is calculated according to eq (10), where ($k < j$). Again, if the selection involves volume fractions, two volume fractions must be selected to undergo variation, that which is associated with $\hat{f}_j$, as given by eq (10), is written to the file X.PLOT. The model parameter is selected by setting the (froz/vary) switch to '1' in X.DAT. The unit of measure is degree per unit of the 'vary' model parameter.

5, request the program to calculate partial derivatives of (Δ, ψ) with respect to the angle of incidence, ϕ . The measure is unitless, i.e., degree per degree.

6, requests the program to calculate partial derivatives of (Δ, ψ) with respect to the photon energy of light. The unit of measure is degree per electron-volt.

Two things are yet unspecified; both are associated with the last set of options mentioned immediately above. These are presented in succession.

The first is associated with option '1.' One must select or specify one of the effective media for evaluation on the grid of photon energies. Accordingly, the program prompts the user with the following:

```
Enter:  kmix " effective medium of dielectric function
```

Here, one enters an integer for the index label of the appropriate effective medium, i.e., ($1 \leq \text{kmix} \leq m_{\text{media}}$) as discussed in section 4.2.5.

The second thing yet unspecified is the grid of source variables, the classical optical frequencies (or the wavelengths in vacuum or associated photon energies) and the angles of incidence, i.e., (λ, ϕ) . Since the grid is constructed from a set of nested DO-loops, one specifies the grid by specifying three numerical values, i.e., the lower bound, the upper bound, and the stepsize, for each axis or dimension of the grid. The program prompts the user for each axis individually. These input values are check-tested, as appropriate. See section 6.2.5, subroutine SCATOI.

The first prompt-request is the following:

```
Enter:  range of incident energies (eV)
or:      - wavelengths (nm)
Enter:  ev1, ev2, ev3
```

where *ev1* is the lower bound, *ev2* is the upper bound, and *ev3* is the stepsize. Negative values are associated with wavelength in units of nanometers, and positive values are associated with energy in units of electron-volts.

Following an answer to the above prompt, the program issues the second prompt-request:

```
Enter:   range of incident angles (degrees)
Enter:   angle1, angle2, angle3
```

where *angle1* is the lower bound, *angle2* is the upper bound, and *angle3* is the stepsize.

Incidentally, the field quantities are written to the output file X.PLOT from either of two subroutines, i.e., SCATO1 or SCATO2, depending upon the set of ordered pairs (λ, ϕ) that is selected at level two, i.e., input from measurements in X.DAT or some discrete grid of values. Regarding these two subroutines, their use of suggestive names for variables, as well as from the lines of comments that are enclosed within the various subroutines, it ought to be rather straightforward for the user to add his own selection of field quantities to the program. This completes the list of options available to the user regarding calculations of the direct or forward problem and graphics.

4.3.2 Search (vary)

Following the selection of option '2' at level one, the main program calls the subroutine SEEKO1 to invert the ellipsometric equations, thus entering level two, see section 6.2.10. This subroutine initiates and maintains the search for a minimum to the error expression as an unconstrained optimization problem, as discussed in section 3.1. The (froz/vary) switch specifies the model parameters which have numerical values that are undergoing variation. At least one numerical value must undergo variation per measurement of (Δ, ψ) , so that the associated rows in the Jacobian are not zero. Note that an iterative method requires an initial solution. Here, the initial value solution is given by the initial input of model parameters as presented in section 4.2. The problem is now completely defined; no further specifications are necessary; no further menus need to be issued to the user.

Since the optimization algorithm is unconstrained, unphysical fixed-point solutions are possible and likely during analyses. These pseudo solutions were discussed earlier in section 3.

The following presents a brief orientation regarding the internal organization of the subroutine SEEKO1. The organization is that for setting up an iterative loop. It calls subroutine ASMBL to construct the Jacobian matrix. It calls subroutine CGNL to solve for the Newton step. It updates the numerical value of the selected model parameters and tests the rate of reduction of the *error* expression. The progress regarding the rate of reduction is written to the output file, X.OUT. If the rate of reduction is sufficiently small to merit no further expenditure, it returns; otherwise, it continues iterating. Such calculations usually involve short durations of time, thus breakpointing is not necessary, and so it was not incorporated into the routine.

Upon completion of the above exercises, the program reports its *best* fixed-point solution. The deviations between the measurement data and that of the model are written to the plot file, X.PLOT, using subroutine SCATO1.

Statistics regarding the deviations are provided by subroutine STAT22. It reports the statistical means, standard deviations, and the correlation coefficient of the deviations, i.e.,

$$g_{\Delta,i} = \Delta_i^e - \Delta_i^m \quad \text{and} \quad g_{\psi,i} = \psi_i^e - \psi_i^m,$$

which is distinct from eqs (12) and (13) from section 3.1. Here, the deviations involve no scaling by the measurement uncertainties. The estimated mean for Δ is defined by

$$\langle g_{\Delta} \rangle \equiv \frac{1}{M} \sum_{i=1}^M g_{\Delta,i},$$

the estimated variance is defined by

$$\langle (g_{\Delta} - \langle g_{\Delta} \rangle)^2 \rangle \equiv \frac{1}{M} \sum_{i=1}^M (g_{\Delta,i} - \langle g_{\Delta} \rangle)^2,$$

where the square root estimates the standard deviation, the covariance is defined by

$$\langle (g_{\Delta} - \langle g_{\Delta} \rangle) (g_{\psi} - \langle g_{\psi} \rangle) \rangle \equiv \frac{1}{M} \sum_{i=1}^M (g_{\Delta,i} - \langle g_{\Delta} \rangle) (g_{\psi,i} - \langle g_{\psi} \rangle),$$

and the correlation coefficient is defined by the ratio formed by the covariance divided by the product of standard deviations of $g_{\Delta,i}$ and $g_{\psi,i}$.

In regards to providing an analysis of sensitivities, here too, the Jacobian involves no row scaling by the measurement uncertainties. Similarly, a scaling matrix $\mathbf{S}$ is then defined. A

correlation matrix, defined by $[\tilde{\mathbf{J}}^T \tilde{\mathbf{J}}]$, is calculated by subroutine CORLAT. Being a symmetric matrix, only the upper triangle is reported. The output file reports the condition number of this matrix. The diagonal elements of the scaling matrix are reported as well. Such reports help identify which model parameters may be correlated, and aid the decision process regarding the selection of frozen model parameters for a series of calculations.

Lastly, the output file reports the estimated uncertainties of the 'vary' model parameters as calculated from eq (22) in section 3.2. Following these exercises, the program stops.

4.3.3 Search Grid (vary)

After the selection of option '3' at level one, the main program calls subroutine SCANO2 to invert the ellipsometric equations, thus entering level two, see section 6.2.9. This subroutine seeks to find a minimum to the error expression, as a constrained optimization problem, by initiating a scan over a grid of numerical values associated with a selected set of model parameters. Here, the (froz/vary) switch specifies the selection; the model parameters contributing to the grid are those whose numerical values are selected to undergo variation. Since the grid is constructed from a single block of nested DO-loops, each selected model parameter contributes one independent axis or dimension to the grid, i.e., a hyper-cube, apart from the special consideration that is necessary for the volume fractions. Note that efficient use of the grid occurs only when the selected model parameters are common to all samples.

Each independent axis of the grid involves four items: the local index label for the model parameter, the lower bound, the upper bound, and the stepsize. To provide this information to the program, it is convenient to follow the convention of DO-loop specification and require that the input format be of the form:

$$i_p, p_1, p_2, p_3,$$

where i_p refers to the local index label of the model parameter p , and p_j refers to the numerical value of the model parameter associated with the initial value, final value, and stepsize, respectively.

To enter the DO-loop specification parameters, the parameters are entered in the same order that they occur in the file X.DAT. From section 4.2, the parameters are grouped and ordered as follows: thicknesses, supplementary parameters, and then volume fractions.

Within each group, the model parameters are indexed locally. By adhering to this group ordering and using only local indices, one is able to specify the necessary vary model parameters. Here, i_p refers to the local index label as used in file X.DAT.

Note that while the effective media are indexed as ordered in file X.DAT, the volume fractions are indexed locally from *within* the effective medium, i.e., starting with one. Hence, ($i_p = 2$) could refer to the second volume fraction of any effective medium. This is checked upon input for consistency.

Regarding volume fractions and eq (10) from section 2.3, it is assumed that k refers to the smallest local index label among those selected to undergo variation for that particular effective medium. DO-loop specification parameters are *not* allowed for f_k , but are required for those f_j selected for optimization, i.e., ($k < j$).

In regard to these considerations, the program issues forth the following lines:

```
Scan a grid of model parameters: (z,p,f).
Grid info:   DO-loop parameters
Grid info:   i,          initial,      final,      increment
```

For each point on the multidimensional grid of model parameters, the program is designed to provide either one of two things. It may simply evaluate the residual at each grid point, and then compare values of the residual over the entire grid. Here, the *best* solution yields the smallest residual. The Jacobian is not calculated. Although small stepsizes are often requested, this may be a relatively fast calculation.

Alternatively, the calculation may initiate a series of unconstrained optimization problems using the Jacobian, except that the range of numerical values of the selected model parameters is restricted to remain within the bounds of the grid. At the conclusion of the grid scan, the program reports its *best* fixed-point solution. The program also reports any components of the solution that lie near the boundary of the selected grid. Solutions with components at grid boundaries are, of course, grid dependent, and as such, further calculation is usually necessary, i.e., after the grid is moved or redefined. Again, the calculations involve the Jacobian. Although large stepsizes are often requested, this may be a relatively slow calculation.

In regard to these considerations, the program presents the following menu of options:

Enter: option regarding the grid scan:
0, no optimization, |g| only,
1, full optimization, Jacobian.

The format convention for indicating the type of optimization is of the form:

$$i_o$$

where i_o is an integer with value 0 or 1, accordingly.

Since the grid specification includes the stepsize, the calculations may become very time-consuming. For this reason, the program writes breakpoint information to the output file X.SOUT at intervals of 15 cpu-minutes. This is discussed in section 4.1.1. The procedure for restarting a previously interrupted calculation is rather straightforward. One need merely append the contents of X.SOUT onto the end of the input data file X.INN, *without* any intervening blank lines. Upon starting any grid scan calculation, the program will attempt to read a set of breakpoint information. If restarting is not intended by the user, the input data file ought to be absent of excess lines. The program does initiate some measure of check-testing regarding the breakpoint information. Anything deemed irregular in the input file should inhibit the chances of erroneous restarts, but it is good practice to truncate the input data file with either an end-of-file condition or some other delimiter, e.g., a short line of connected equal signs.

Again, as presented in the previous subsection, i.e., section 4.3.2, the program reports a few basic statistics regarding deviations of the fit between the measurement data and that of the model, as well as the estimated uncertainties in the model parameters.

5. Worked Examples

The following subsections present worked examples using the program. Each subsection presents an example involving one selection from among the set of available top level options. A brief orientation is given regarding the purpose of each calculation. Since the program outputs a journal listing of the input data, only the output file needs to be presented in the following subsections. Again, an example of the input file X.DAT may be found in section 4.2.9. For convenience, the input file X.INN is included as well. The input/output files are shown as indexed for convenience.

5.1 Forward Problems, Plots, ...

This option is discussed in sections 4.3 and 4.3.1. Consider again the example that is presented in section 4.2.9. The input file X.DAT contains both the characterization of the sample and the measurement data of ellipsometric angles. For the sake of demonstration, suppose that only the characterization of the sample is known. Let the exercise here be that of generating a set of measurement data. A suitable input file X.DAT may be as follows:

```

1 drb1:[data_bases]w.
2 -----
3 2                                ! mfilmz " thicknesses /(i,z,zu,ivary)
4 1 100.0 2.0 0                  ! i,z,zu,ivary " top layer, SiO2
5 2 2.0 2.0 0                  ! i,z,zu,ivary " bottom layer, SiO2+Si
6 -----
7 0                              ! mipars / (i,ip)
8 -----
9 0                              ! mrpars / (i,rp,up,ivary)
10 -----
11 4                              ! mixtures " number of effective media
12 1 0 0                          ! mlmnt,mipar,mrpar #1
13 1 2 1.0 0.0 0                ! j,lmnt,frac,ufrac,ivary " air
14 1 0 0                          ! mlmnt,mipar,mrpar #2
15 1 3 1.0 0.0 0                ! j,lmnt,frac,ufrac,ivary " Si
16 1 0 0                          ! mlmnt,mipar,mrpar #3
17 1 5 1.0 0.0 0                ! j,lmnt,frac,ufrac,ivary " SiO2
18 2 0 0                          ! mlmnt,mipar,mrpar #4
19 1 3 0.5 0.02 1              ! j,lmnt,frac,ufrac,ivary " Si
20 2 5 0.5 0.02 1              ! j,lmnt,frac,ufrac,ivary " SiO2
21 -----
22 1                              ! mbient " number of ambients
23 1 1 0 0                      ! j,imix,mipar,mrpar " air
24 -----
25 1                              ! msampl " number of samples analyzed

```



```

26  2          ! mfilm " number of layers on sample #1
27    1  3  1    ! j,imix,iz " SiO2 , top layer
28    2  4  2    ! j,imix,iz " SiO2+Si, transition region
29    3  2          ! j,imix " Si , substrate
30 -----
31  1          ! mbien " number of ambients on sample #1
32  1  1          ! mrpeat,mbien
33    1          ! mexpt " number of measurements
34    1    1.5    70.0    0.0    0.0          (i,E,a, d,p)
35          0.1    0.01    0.01    0.01      (uncertainty)

```

Note, the above last two lines involve pseudo measurement data. Also, only two volume fractions are shown selected for variation, i.e., lines 19 and 20. Due to the constraint among volume fractions for an effective medium, only one variable is subject to optimization, i.e., the oxide. This is mentioned in section 4.3.1 in option 4 near the bottom of page 43.

Suppose now that measurement data are requested for optical frequencies which correspond to energies between 1.5 and 6.0 eV with stepsize of 0.5 eV. Further, let this involve only one angle of incidence, e.g., 70 deg. A suitable input file X.INN may be as follows:

```

1  1          ! forward problems, plots, ...
2  2          ! grid scan
3  2          ! (Delta, psi), x.dat
4  1.5    6.0    0.5    ! grid energy (eV)
5  70.    70.    0.0    ! grid angle of incidence (degrees)

```

Given the above two input files, the program generates two output files. The output file X.OUT contains a journal listing of the program's activity. The output file X.OUT is given below.

```

1  Enter:  sub-directory    for constituent media
2          sub-directory " drb1:[data_bases]w.
3
4  -----
5  Enter:  mfilmz " number of distinct widths
6    2      mfilmz " number of distinct widths
7  Enter:  i,z,zu,ivary
8    1  100.000    2.000    0    i,z,zu,ivary
9    2    2.000    2.000    0    i,z,zu,ivary
10
11 -----
12 Enter:  mipars " number of parameters (integer)
13    0      mipars " number of parameters (integer)
14
15 -----

```

```

16 Enter:      mrpars " number of parameters (floating-point)
17   0        mrpars " number of parameters (floating-point)
18
19 -----
20 Enter:      mmixtr " number of distinct mixtures
21   4        mmixtr " number of distinct mixtures
22
23 Enter:      mlmnt, mipar, mrpar      (mix # 1)
24   1  0  0   mlmnt, mipar, mrpar
25 Enter:      j, lmnt, frac, ufrac, ivary
26   1  2  1.00000  0.00000  0   j, lmnt, frac, ufrac, ivary
27
28 Enter:      mlmnt, mipar, mrpar      (mix # 2)
29   1  0  0   mlmnt, mipar, mrpar
30 Enter:      j, lmnt, frac, ufrac, ivary
31   1  3  1.00000  0.00000  0   j, lmnt, frac, ufrac, ivary
32
33 Enter:      mlmnt, mipar, mrpar      (mix # 3)
34   1  0  0   mlmnt, mipar, mrpar
35 Enter:      j, lmnt, frac, ufrac, ivary
36   1  5  1.00000  0.00000  0   j, lmnt, frac, ufrac, ivary
37
38 Enter:      mlmnt, mipar, mrpar      (mix # 4)
39   2  0  0   mlmnt, mipar, mrpar
40 Enter:      j, lmnt, frac, ufrac, ivary
41   1  3  0.50000  0.02000  1   j, lmnt, frac, ufrac, ivary
42   2  5  0.50000  0.02000  1   j, lmnt, frac, ufrac, ivary
43
44 -----
45 Enter:      mbient " number of distinct ambients
46   1        mbient " number of distinct ambients
47 Enter:      j, imix, mipar, mrpar
48   1  1  0  0   j, imix, mipar, mrpar
49
50 -----
51 Enter:      msampl " number of samples
52   1        msampl " number of samples
53
54 Enter:      mfilm " number of films on sample # 1
55   2        mfilm " number of films on sample # 1
56 Enter:      j, imix, iwidth      (film/substrate)
57   1  3  1   j, imix, iwidth
58   2  4  2   j, imix, iwidth
59   3  2   j, imix
60
61 -----
62 Enter:      mbien " number of ambients on sample # 1
63   1        mbien " number of ambients on sample # 1
64 Enter:      mrpeat, imbien
65   1  1   mrpeat, imbien
66 Enter:      mexpt " number of measurement data
67   1        mexpt " number of measurement data
68 Enter:      j, wavln (nm), angln,delta,psi (degree)

```

```

69          wavlno      , anglu,deltu,psiu
70
71      1      1.500      70.000      0.000      0.000      (j, wavlno,angli, delta,psi )
72          0.100      0.010      0.010      0.010      ( wavlno,anglu, deltu,psiu)
73
74
75  Enter:  option
76          1, forward problems, plots, ...
77          2, search      (vary)
78          3, search grid (vary)
79  option =  1
80
81
82  Enter:  choice of incident (energies, angles)
83          1, measurement data,      x.dat
84          2, grid scan.
85  choice =  2
86
87  Enter:  choice of output suitable for:
88          1, dielectric function, media,
89          2, (Delta, psi),      x.dat,
90          3, (Delta, psi),      plotting,
91          4, d/db,      b*(z,f,p),
92          5, d/da,      angle of incidence,
93          6, d/dE,      energy.
94  choice =  2
95
96  Enter:  range of incident energies (eV)
97  or:      - wavelengths (nm)
98  Enter:  ev1, ev2, ev3
99          1.5000      6.0000      0.5000      energy (eV)
100
101  Enter:  range of incident angles (degrees)
102  Enter:  angle1, angle2, angle3
103          70.0000      70.0000      0.0000      a1,a2,a3
104
105  lmnt = 2, filename = air
106  lmnt = 5, filename = Si_O2g
107  lmnt = 3, filename = Si
108
109  elapsed cpu-time = 37 centi-seconds
110                  + 1 seconds

```

Again, three constituent media are used in these calculations, and 'lmnt' is a mnemonic for *elements* or constituents. Regarding the constituent media of air, crystalline silicon, and amorphous silicon dioxide, their index labels are given by 2, 3, and 5, respectively. This is shown above on lines 105 to 107.

The output file X.PLOT contains the requested set of measurement data of ellipsometric

angles, (Δ, ψ) . The output file X.PLOT is given below.

```

1      1      msampl
2      1      mbien
3      1      1      mrpeat, imbien
4      10      mexpt " measurements
5      1      1.50000E+00  7.00000E+01  8.04309E+01  3.08875E+01 (i,E,a, d,p)
6      1      1.00000E-01  1.00000E-02  1.00000E-02  1.00000E-02 (uncertainty)
7      2      2.00000E+00  7.00000E+01  7.97129E+01  4.31275E+01 (i,E,a, d,p)
8      2      1.00000E-01  1.00000E-02  1.00000E-02  1.00000E-02 (uncertainty)
9      3      2.50000E+00  7.00000E+01  1.02227E+02  6.93018E+01 (i,E,a, d,p)
10     3      1.00000E-01  1.00000E-02  1.00000E-02  1.00000E-02 (uncertainty)
11     4      3.00000E+00  7.00000E+01  2.50415E+02  6.09989E+01 (i,E,a, d,p)
12     4      1.00000E-01  1.00000E-02  1.00000E-02  1.00000E-02 (uncertainty)
13     5      3.50000E+00  7.00000E+01  2.62427E+02  4.00376E+01 (i,E,a, d,p)
14     5      1.00000E-01  1.00000E-02  1.00000E-02  1.00000E-02 (uncertainty)
15     6      4.00000E+00  7.00000E+01  2.47313E+02  3.31054E+01 (i,E,a, d,p)
16     6      1.00000E-01  1.00000E-02  1.00000E-02  1.00000E-02 (uncertainty)
17     7      4.50000E+00  7.00000E+01  1.92800E+02  3.34557E+01 (i,E,a, d,p)
18     7      1.00000E-01  1.00000E-02  1.00000E-02  1.00000E-02 (uncertainty)
19     8      5.00000E+00  7.00000E+01  1.24499E+02  3.21867E+01 (i,E,a, d,p)
20     8      1.00000E-01  1.00000E-02  1.00000E-02  1.00000E-02 (uncertainty)
21     9      5.50000E+00  7.00000E+01  8.77637E+01  3.66717E+01 (i,E,a, d,p)
22     9      1.00000E-01  1.00000E-02  1.00000E-02  1.00000E-02 (uncertainty)
23    10      6.00000E+00  7.00000E+01  7.10687E+01  4.18238E+01 (i,E,a, d,p)
24    10      1.00000E-01  1.00000E-02  1.00000E-02  1.00000E-02 (uncertainty)

```

The data in file X.PLOT may then be inserted into file X.DAT, i.e., replacing the previous pseudo measurement data, see sections 4.2.8 and 4.2.9. This concludes one method or procedure that may be used for generating model measurement data.

5.2 Search (vary)

This option is discussed in sections 4.3 and 4.3.2 regarding the inverse problem. Suppose now that one is given the ellipsometric measurement data. For convenience, let the measurements be those presented in section 5.1. Since the inverse problem involves determining the model parameters from the measurements, let the initial solution be close to the true solution. Regarding the transition region of the sample, let the volume fractions be displaced from their correct values. Let the volume fraction for the silicon be judiciously set to 0.7, see line 19 below.

Further, let only one variable be subjected to optimization, and let it involve only the volume fractions of the transition region. The purpose here is to show the rate of convergence of the program. Attention is directed less toward optimality of iterations than that which is necessary to follow convergence. Again, the measurement data are exact for the correct model parameters, the system is nicely overdetermined, and the correct solution is found. The input file X.DAT is given below:

```

1  drb1:[data_bases]w.
2  -----
3  2                      ! mfilmz " thicknesses /(i,z,zu,ivary)
4  1    100.0    2.0    0    ! i,z,zu,ivary " top layer, SiO2
5  2      2.0    2.0    0    ! i,z,zu,ivary " bottom layer, SiO2+Si
6  -----
7  0                      ! mipars / (i,ip)
8  -----
9  0                      ! mrpars / (i,rp,up,ivary)
10 -----
11 4                      ! mixtures " number of effective media
12 1 0 0                  ! mlmnt,mipar,mrpar #1
13 1 2 1.0 0.0 0          ! j,lmnt,frac,ufrac,ivary " air
14 1 0 0                  ! mlmnt,mipar,mrpar #2
15 1 3 1.0 0.0 0          ! j,lmnt,frac,ufrac,ivary " Si
16 1 0 0                  ! mlmnt,mipar,mrpar #3
17 1 5 1.0 0.0 0          ! j,lmnt,frac,ufrac,ivary " SiO2
18 2 0 0                  ! mlmnt,mipar,mrpar #4
19 1 3 0.7 0.02 1         ! j,lmnt,frac,ufrac,ivary " Si
20 2 5 0.3 0.02 1         ! j,lmnt,frac,ufrac,ivary " SiO2
21 -----
22 1                      ! mbient " number of ambients
23 1 1 0 0                ! j,imix,mipar,mrpar " air
24 -----
25 1                      ! msampl " number of samples analyzed
26 2                      ! mfilm " number of layers on sample #1
27 1 3 1                  ! j,imix,iz " SiO2 , top layer
28 2 4 2                  ! j,imix,iz " SiO2+Si, transition region

```

```

29      3  2      !      j,imix      " Si      , substrate
30      -----
31      1      ! mbien " number of ambients on sample #1
32      1  1      ! mrpeat,imbien
33      10      ! mexpt " number of measurements
34      1      1.50000E+00  7.00000E+01  8.04309E+01  3.08875E+01 (i,E,a, d,p)
35      1.00000E-01  1.00000E-02  1.00000E-02  1.00000E-02 (uncertainty)
36      2      2.00000E+00  7.00000E+01  7.97129E+01  4.31275E+01 (i,E,a, d,p)
37      1.00000E-01  1.00000E-02  1.00000E-02  1.00000E-02 (uncertainty)
38      3      2.50000E+00  7.00000E+01  1.02227E+02  6.93018E+01 (i,E,a, d,p)
39      1.00000E-01  1.00000E-02  1.00000E-02  1.00000E-02 (uncertainty)
40      4      3.00000E+00  7.00000E+01  2.50415E+02  6.09989E+01 (i,E,a, d,p)
41      1.00000E-01  1.00000E-02  1.00000E-02  1.00000E-02 (uncertainty)
42      5      3.50000E+00  7.00000E+01  2.62427E+02  4.00376E+01 (i,E,a, d,p)
43      1.00000E-01  1.00000E-02  1.00000E-02  1.00000E-02 (uncertainty)
44      6      4.00000E+00  7.00000E+01  2.47313E+02  3.31054E+01 (i,E,a, d,p)
45      1.00000E-01  1.00000E-02  1.00000E-02  1.00000E-02 (uncertainty)
46      7      4.50000E+00  7.00000E+01  1.92800E+02  3.34557E+01 (i,E,a, d,p)
47      1.00000E-01  1.00000E-02  1.00000E-02  1.00000E-02 (uncertainty)
48      8      5.00000E+00  7.00000E+01  1.24499E+02  3.21867E+01 (i,E,a, d,p)
49      1.00000E-01  1.00000E-02  1.00000E-02  1.00000E-02 (uncertainty)
50      9      5.50000E+00  7.00000E+01  8.77637E+01  3.66717E+01 (i,E,a, d,p)
51      1.00000E-01  1.00000E-02  1.00000E-02  1.00000E-02 (uncertainty)
52      10     6.00000E+00  7.00000E+01  7.10687E+01  4.18238E+01 (i,E,a, d,p)
53      1.00000E-01  1.00000E-02  1.00000E-02  1.00000E-02 (uncertainty)

```

The option for unconstrained optimization is selected by setting the one and only line of data in the input file X.INN to the integer value 2, i.e.,

```

1  2      ! search (vary)

```

The output file X.OUT contains a journal listing of the input data, progress reports regarding convergence, the final numerical values of the vary model parameters, and a selection of associated statistics, as well as the amount of cpu-time that is used during calculation. The output shows on line 132 that 27 iterations were used to converge to the correct final solution shown on line 135. Again, regarding line 135, the index label 5 refers to the volume fraction for amorphous silicon dioxide. This index label refers to the fifth successive volume fraction found by cumulative indexing the constituent media of the effective media, and not the constituent label xx that would be associated with DIELxx. The output file X.OUT is given below.

```

1  Enter:  sub-directory      for constituent media
2          sub-directory " drbi:[data_bases]w.
3

```

```

4 -----
5 Enter:      mfilmz " number of distinct widths
6      2      mfilmz " number of distinct widths
7 Enter:      "      i,z,zu,ivary
8      1      100.000      2.000      0      i,z,zu,ivary
9      2      2.000      2.000      0      i,z,zu,ivary
10
11 -----
12 Enter:      mipars " number of parameters (integer)
13      0      mipars " number of parameters (integer)
14
15 -----
16 Enter:      mrpars " number of parameters (floating-point)
17      0      mrpars " number of parameters (floating-point)
18
19 -----
20 Enter:      mmixtr " number of distinct mixtures
21      4      mmixtr " number of distinct mixtures
22
23 Enter:      mlmnt, mipar, mrpar      (mix # 1)
24      1      0      0      mlmnt, mipar, mrpar
25 Enter:      "      j, lmnt, frac, ufrac, ivary
26      1      2      1.00000      0.00000      0      j, lmnt, frac, ufrac, ivary
27
28 Enter:      mlmnt, mipar, mrpar      (mix # 2)
29      1      0      0      mlmnt, mipar, mrpar
30 Enter:      "      j, lmnt, frac, ufrac, ivary
31      1      3      1.00000      0.00000      0      j, lmnt, frac, ufrac, ivary
32
33 Enter:      mlmnt, mipar, mrpar      (mix # 3)
34      1      0      0      mlmnt, mipar, mrpar
35 Enter:      "      j, lmnt, frac, ufrac, ivary
36      1      5      1.00000      0.00000      0      j, lmnt, frac, ufrac, ivary
37
38 Enter:      mlmnt, mipar, mrpar      (mix # 4)
39      2      0      0      mlmnt, mipar, mrpar
40 Enter:      "      j, lmnt, frac, ufrac, ivary
41      1      3      0.70000      0.02000      1      j, lmnt, frac, ufrac, ivary
42      2      5      0.30000      0.02000      1      j, lmnt, frac, ufrac, ivary
43
44 -----
45 Enter:      mbient " number of distinct ambients
46      1      mbient " number of distinct ambients
47 Enter:      "      j, imix, mipar, mrpar
48      1      1      0      0      j, imix, mipar, mrpar
49
50 -----
51 Enter:      msampl " number of samples
52      1      msampl " number of samples
53
54 Enter:      mfilm " number of films on sample # 1
55      2      mfilm " number of films on sample # 1
56 Enter:      "      j, imix, iwidth      (film/substrate)

```

```

57      1      3      1      j, imix, iwidth
58      2      4      2      j, imix, iwidth
59      3      2              j, imix
60
61 -----
62 Enter:      mbien " number of ambients on sample # 1
63      1      mbien " number of ambients on sample # 1
64 Enter:      mrpeat, imbien
65      1      1      mrpeat, imbien
66 Enter:      mexpt " number of measurement data
67      10      mexpt " number of measurement data
68 Enter:      j, wavln (nm), angli,delta,psi (degree)
69              wavlnu      , anglu,deltu,psiu
70
71      1      1.500      70.000      80.431      30.888      (j, wavln,angli, delta,psi )
72              0.100      0.010      0.010      0.010      ( wavlu,anglu, deltu,psiu)
73      2      2.000      70.000      79.713      43.127      (j, wavln,angli, delta,psi )
74              0.100      0.010      0.010      0.010      ( wavlu,anglu, deltu,psiu)
75      3      2.500      70.000      102.227      69.302      (j, wavln,angli, delta,psi )
76              0.100      0.010      0.010      0.010      ( wavlu,anglu, deltu,psiu)
77      4      3.000      70.000      250.415      60.999      (j, wavln,angli, delta,psi )
78              0.100      0.010      0.010      0.010      ( wavlu,anglu, deltu,psiu)
79      5      3.500      70.000      262.427      40.038      (j, wavln,angli, delta,psi )
80              0.100      0.010      0.010      0.010      ( wavlu,anglu, deltu,psiu)
81      6      4.000      70.000      247.313      33.105      (j, wavln,angli, delta,psi )
82              0.100      0.010      0.010      0.010      ( wavlu,anglu, deltu,psiu)
83      7      4.500      70.000      192.800      33.456      (j, wavln,angli, delta,psi )
84              0.100      0.010      0.010      0.010      ( wavlu,anglu, deltu,psiu)
85      8      5.000      70.000      124.499      32.187      (j, wavln,angli, delta,psi )
86              0.100      0.010      0.010      0.010      ( wavlu,anglu, deltu,psiu)
87      9      5.500      70.000      87.764      36.672      (j, wavln,angli, delta,psi )
88              0.100      0.010      0.010      0.010      ( wavlu,anglu, deltu,psiu)
89      10      6.000      70.000      71.069      41.824      (j, wavln,angli, delta,psi )
90              0.100      0.010      0.010      0.010      ( wavlu,anglu, deltu,psiu)
91
92
93 Enter:      option
94              1, forward problems, plots, ...
95              2, search      (vary)
96              3, search grid (vary)
97 option =      2
98
99 lmnt "      2, filename = air
100 lmnt "      5, filename = Si_02g
101 lmnt "      3, filename = Si
102
103 seek:      loop,      ratio of reduction,      |g|
104              (rel)      (total)
105              0              1.268E+02
106              1      8.800E-01      8.800E-01      1.116E+02
107              2      8.668E-01      7.628E-01      9.670E+01
108              3      8.508E-01      6.490E-01      8.227E+01
109              4      8.308E-01      5.392E-01      6.836E+01

```



```

110      5      8.050E-01      4.341E-01      5.503E+01
111      6      7.702E-01      3.343E-01      4.238E+01
112      7      7.200E-01      2.407E-01      3.051E+01
113      8      6.388E-01      1.538E-01      1.949E+01
114      9      6.143E-01      9.446E-02      1.197E+01
115     10      6.093E-01      5.755E-02      7.295E+00
116     11      6.056E-01      3.485E-02      4.418E+00
117     12      6.039E-01      2.105E-02      2.668E+00
118     13      6.020E-01      1.267E-02      1.606E+00
119     14      6.012E-01      7.618E-03      9.657E-01
120     15      6.019E-01      4.585E-03      5.813E-01
121     16      6.003E-01      2.753E-03      3.489E-01
122     17      6.037E-01      1.662E-03      2.107E-01
123     18      6.001E-01      9.972E-04      1.264E-01
124     19      6.082E-01      6.065E-04      7.688E-02
125     20      6.108E-01      3.704E-04      4.696E-02
126     21      6.391E-01      2.367E-04      3.001E-02
127     22      6.788E-01      1.607E-04      2.037E-02
128     23      7.420E-01      1.192E-04      1.512E-02
129     24      8.563E-01      1.021E-04      1.294E-02
130     25      9.337E-01      9.535E-05      1.209E-02
131     26      9.660E-01      9.211E-05      1.168E-02
132     27      9.638E-01      8.877E-05      1.125E-02
133
134 model parameter value along the minimum:
135      1)      0.5000      0.00000,      for:      5 " (f,fu)
136
137 initial |g| = 1.26767E+02
138 final |g| = 1.12530E-02
139
140 -----
141 Statistics of deviations " experiment-model " g
142
143 where: g is a column vector of length 2M,
144      () denotes either (delta) or (psi)
145 mean () = m() = <g()> = (1/M) sum: g()
146 variance () = < (g() -m()) **2 >
147 covariance = < (g(1)-m(1))*(g(2)-m(2)) >
148 std dev = sqrt (variance)
149 correlat coef = covariance / (sd(1) * sd(2))
150
151      mean,      std dev      (degrees)
152 psi:      0.000      0.000
153 delta:      0.000      0.000
154      0.172 " correlation coefficient " <psi|delta>
155
156 [J(T)*J], renormalized for correlation.
157      1)      1.00000
158
159 Normalization coefficients, sqrt: [J(T)*J]_(i,i)
160      7.80E-02
161
162 rcond = 1.00E+00, condition number, [J(T)*J]

```

```

163
164 [J(T)*J]**(-1):
165     Determinant:      10.0000 E -1.0000
166     Inertia:   (  1  0  0), number of (+,-,0) eigenvalues.
167     Inverse:    upper+diagonal matrix
168     1)    1.00E+00
169
170 -----
171 The standard deviation of the residuals.
172
173 s(g) = sqrt [<gg>/((2M-N))] =  1.15453E-04 (degrees)
174
175
176 The estimated uncertainty in the model parameters,
177 assuming no correlation, i.e., diagonal terms only.
178
179             value,    uncertainty.
180     1)      0.5000      0.00003,   for:    5 " (f,fu)
181
182 elapsed cpu-time = 10 centi-seconds
183                  + 10 seconds

```

Note that lines 137 and 138 refer to root-mean-square (rms) residuals, which involve deviations scaled by the measurement uncertainties, and hence, are unitless. The final rms residual is near 10^{-2} , and the measurement uncertainty is 10^{-2} . Hence, the final rms deviation is near 10^{-4} , as is shown on line 173.

The output file X.PLOT contains a listing of the deviations between the measurements of (Δ, ψ) and that calculated for the model. The output file X.PLOT is presented below.

1	1	msampl					
2	1	mbien					
3	1	1	mrpeat, imbien				
4	10	2	mexpt, mu				
5	1	1.50000E+00	7.00000E+01	0.00000E+00	6.83019E-06	(i,E,a	g (d,p))
6	2	2.00000E+00	7.00000E+01	5.46415E-05	-4.09811E-05	(i,E,a	g (d,p))
7	3	2.50000E+00	7.00000E+01	1.36604E-04	-1.02453E-04	(i,E,a	g (d,p))
8	4	3.00000E+00	7.00000E+01	-4.78113E-05	2.04906E-05	(i,E,a	g (d,p))
9	5	3.50000E+00	7.00000E+01	-2.59547E-04	-3.07358E-05	(i,E,a	g (d,p))
10	6	4.00000E+00	7.00000E+01	3.21019E-04	5.12264E-05	(i,E,a	g (d,p))
11	7	4.50000E+00	7.00000E+01	-5.46415E-05	1.36604E-05	(i,E,a	g (d,p))
12	8	5.00000E+00	7.00000E+01	1.91245E-04	1.02453E-05	(i,E,a	g (d,p))
13	9	5.50000E+00	7.00000E+01	0.00000E+00	3.41509E-05	(i,E,a	g (d,p))
14	10	6.00000E+00	7.00000E+01	0.00000E+00	-4.09811E-05	(i,E,a	g (d,p))

5.3 Search Grid (vary)

This option is discussed in sections 4.3 and 4.3.3. Suppose again that the exercise of the single search that was presented in the previous subsection yielded a residual much larger than the measurement uncertainties, and yet there is strong conviction that the model is reasonable. One may then want to find the *best* solution that is available for this given model of the sample. Hence, one may be led to consider searching a grid of model parameters.

Regarding the example presented in the previous section, suppose further that the thickness of the transition region is sought as well. For convenience, let the initial value solution be displaced from the correct value; let the thickness be set to 3 nm, see line 5. The input file X.DAT is given below.

```

1  drb1:[data_bases]w.
2  -----
3  2                                ! mfilmz ~ thicknesses /(i,z,zu,ivary)
4  1    100.0    2.0    0    ! i,z,zu,ivary ~ top layer, SiO2
5  2     3.0    2.0    1    ! i,z,zu,ivary ~ bottom layer, SiO2+Si
6  -----
7  0                                ! mipars / (i,ip)
8  -----
9  0                                ! mrpars / (i,rp,up,ivary)
10 -----
11 4                                ! mixtures ~ number of effective media
12 1 0 0                            ! mlmnt,mipar,mrpar #1
13 1 2 1.0 0.0 0                    ! j,lmnt,frac,ufrac,ivary ~ air
14 1 0 0                            ! mlmnt,mipar,mrpar #2
15 1 3 1.0 0.0 0                    ! j,lmnt,frac,ufrac,ivary ~ Si
16 1 0 0                            ! mlmnt,mipar,mrpar #3
17 1 5 1.0 0.0 0                    ! j,lmnt,frac,ufrac,ivary ~ SiO2
18 2 0 0                            ! mlmnt,mipar,mrpar #4
19 1 3 0.7 0.02 1                   ! j,lmnt,frac,ufrac,ivary ~ Si
20 2 5 0.3 0.02 1                   ! j,lmnt,frac,ufrac,ivary ~ SiO2
21 -----
22 1                                ! mbient ~ number of ambients
23 1 1 0 0                          ! j,imix,mipar,mrpar ~ air
24 -----
25 1                                ! msampl ~ number of samples analyzed
26 2                                ! mfilm ~ number of layers on sample #1
27 1 3 1                            ! j,imix,iz ~ SiO2 , top layer
28 2 4 2                            ! j,imix,iz ~ SiO2+Si, transition region
29 3 2                              ! j,imix ~ Si , substrate
30 -----
31 1                                ! mbien ~ number of ambients on sample #1
32 1 1                              ! mrpeat,imbien
33 10                              ! mexpt ~ number of measurements

```

34	1	1.50000E+00	7.00000E+01	8.04309E+01	3.08875E+01	(i,E,a, d,p)
35		1.00000E-01	1.00000E-02	1.00000E-02	1.00000E-02	(uncertainty)
36	2	2.00000E+00	7.00000E+01	7.97129E+01	4.31275E+01	(i,E,a, d,p)
37		1.00000E-01	1.00000E-02	1.00000E-02	1.00000E-02	(uncertainty)
38	3	2.50000E+00	7.00000E+01	1.02227E+02	6.93018E+01	(i,E,a, d,p)
39		1.00000E-01	1.00000E-02	1.00000E-02	1.00000E-02	(uncertainty)
40	4	3.00000E+00	7.00000E+01	2.50415E+02	6.09989E+01	(i,E,a, d,p)
41		1.00000E-01	1.00000E-02	1.00000E-02	1.00000E-02	(uncertainty)
42	5	3.50000E+00	7.00000E+01	2.62427E+02	4.00376E+01	(i,E,a, d,p)
43		1.00000E-01	1.00000E-02	1.00000E-02	1.00000E-02	(uncertainty)
44	6	4.00000E+00	7.00000E+01	2.47313E+02	3.31054E+01	(i,E,a, d,p)
45		1.00000E-01	1.00000E-02	1.00000E-02	1.00000E-02	(uncertainty)
46	7	4.50000E+00	7.00000E+01	1.92800E+02	3.34557E+01	(i,E,a, d,p)
47		1.00000E-01	1.00000E-02	1.00000E-02	1.00000E-02	(uncertainty)
48	8	5.00000E+00	7.00000E+01	1.24499E+02	3.21867E+01	(i,E,a, d,p)
49		1.00000E-01	1.00000E-02	1.00000E-02	1.00000E-02	(uncertainty)
50	9	5.50000E+00	7.00000E+01	8.77637E+01	3.66717E+01	(i,E,a, d,p)
51		1.00000E-01	1.00000E-02	1.00000E-02	1.00000E-02	(uncertainty)
52	10	6.00000E+00	7.00000E+01	7.10687E+01	4.18238E+01	(i,E,a, d,p)
53		1.00000E-01	1.00000E-02	1.00000E-02	1.00000E-02	(uncertainty)

Here, there are three model parameters selected for variation, but only two undergo optimization and contribute to the grid. Both model parameters involve the transition region, the thickness of the layer and the volume fraction for the amorphous silicon dioxide. Regarding the construction of the grid of model parameters: let the thickness range between 1.0 and 3.0 nm with stepsize of 2.0 nm, and let the volume fraction range between 0.3 and 0.7 with stepsize of 0.4, so that no grid point lies on the correct solution. Accordingly, the input file X.INN is given below.

```

1 3                                ! search grid
2 2    1.0    3.0    2.0          ! thickness,                transition region
3 2    0.3    0.7    0.4          ! volume fraction, oxide, transition region
4 1                                ! full optimization, use Jacobian

```

The output file X.OUT is given below.

```

1 Enter:  sub-directory    for constituent media
2         sub-directory " drb1:[data_bases]w.
3
4 -----
5 Enter:  mfilnz " number of distinct widths
6         mfilnz " number of distinct widths
7 Enter:                                i,z,zu,ivary
8         1    100.000    2.000    0    i,z,zu,ivary
9         2     3.000    2.000    1    i,z,zu,ivary
10

```



```

11 -----
12 Enter:      mipars " number of parameters (integer)
13      0      mipars " number of parameters (integer)
14
15 -----
16 Enter:      mrpars " number of parameters (floating-point)
17      0      mrpars " number of parameters (floating-point)
18
19 -----
20 Enter:      mmixtr " number of distinct mixtures
21      4      mmixtr " number of distinct mixtures
22
23 Enter:      mlmnt, mipar, mrpar      (mix # 1)
24      1  0  0  mlmnt, mipar, mrpar
25 Enter:      j, lmnt, frac, ufrac, ivary
26      1  2  1.00000  0.00000  0  j, lmnt, frac, ufrac, ivary
27
28 Enter:      mlmnt, mipar, mrpar      (mix # 2)
29      1  0  0  mlmnt, mipar, mrpar
30 Enter:      j, lmnt, frac, ufrac, ivary
31      1  3  1.00000  0.00000  0  j, lmnt, frac, ufrac, ivary
32
33 Enter:      mlmnt, mipar, mrpar      (mix # 3)
34      1  0  0  mlmnt, mipar, mrpar
35 Enter:      j, lmnt, frac, ufrac, ivary
36      1  5  1.00000  0.00000  0  j, lmnt, frac, ufrac, ivary
37
38 Enter:      mlmnt, mipar, mrpar      (mix # 4)
39      2  0  0  mlmnt, mipar, mrpar
40 Enter:      j, lmnt, frac, ufrac, ivary
41      1  3  0.70000  0.02000  1  j, lmnt, frac, ufrac, ivary
42      2  5  0.30000  0.02000  1  j, lmnt, frac, ufrac, ivary
43
44 -----
45 Enter:      mbient " number of distinct ambients
46      1      mbient " number of distinct ambients
47 Enter:      j, imix, mipar, mrpar
48      1  1  0  0  j, imix, mipar, mrpar
49
50 -----
51 Enter:      msampl " number of samples
52      1      msampl " number of samples
53
54 Enter:      mfilm " number of films on sample # 1
55      2      mfilm " number of films on sample # 1
56 Enter:      j, imix, iwidth      (film/substrate)
57      1  3  1  j, imix, iwidth
58      2  4  2  j, imix, iwidth
59      3  2      j, imix
60
61 -----
62 Enter:      mbien " number of ambients on sample # 1
63      1      mbien " number of ambients on sample # 1

```

```

64 Enter:      mrpeat, imbien
65   1      1      mrpeat, imbien
66 Enter:      mexpt " number of measurement data
67   10      mexpt " number of measurement data
68 Enter:      j, wavln (nm), angli,delta,psi (degree)
69      wavlnu      , anglu,deltu,psiu
70
71   1      1.500      70.000      80.431      30.888      (j, wavln,angli, delta,psi )
72      0.100      0.010      0.010      0.010      ( wavlu,anglu, deltu,psiu)
73   2      2.000      70.000      79.713      43.127      (j, wavln,angli, delta,psi )
74      0.100      0.010      0.010      0.010      ( wavlu,anglu, deltu,psiu)
75   3      2.500      70.000      102.227      69.302      (j, wavln,angli, delta,psi )
76      0.100      0.010      0.010      0.010      ( wavlu,anglu, deltu,psiu)
77   4      3.000      70.000      250.415      60.999      (j, wavln,angli, delta,psi )
78      0.100      0.010      0.010      0.010      ( wavlu,anglu, deltu,psiu)
79   5      3.500      70.000      262.427      40.038      (j, wavln,angli, delta,psi )
80      0.100      0.010      0.010      0.010      ( wavlu,anglu, deltu,psiu)
81   6      4.000      70.000      247.313      33.105      (j, wavln,angli, delta,psi )
82      0.100      0.010      0.010      0.010      ( wavlu,anglu, deltu,psiu)
83   7      4.500      70.000      192.800      33.456      (j, wavln,angli, delta,psi )
84      0.100      0.010      0.010      0.010      ( wavlu,anglu, deltu,psiu)
85   8      5.000      70.000      124.499      32.187      (j, wavln,angli, delta,psi )
86      0.100      0.010      0.010      0.010      ( wavlu,anglu, deltu,psiu)
87   9      5.500      70.000      87.764      36.672      (j, wavln,angli, delta,psi )
88      0.100      0.010      0.010      0.010      ( wavlu,anglu, deltu,psiu)
89  10      6.000      70.000      71.069      41.824      (j, wavln,angli, delta,psi )
90      0.100      0.010      0.010      0.010      ( wavlu,anglu, deltu,psiu)
91
92
93 Enter:      option
94      1, forward problems, plots, ...
95      2, search      (vary)
96      3, search grid (vary)
97 option =      3
98
99
100 Scan a grid of model parameters: (z,p,f).
101 Grid info: DO-loop parameters
102 Grid info: i,      initial,      final,      increment
103
104 Enter:      i, z1, z2, z3      (widths)
105      1)      2      1.0000      3.0000      2.0000      ( 1)
106
107 Enter:      i, f1, f2, f3      (fraction)
108      2)      2      0.3000      0.7000      0.4000      ( 2)
109
110 Enter:      option regarding the grid scan:
111      0, no optimization, |g| only,
112      1, full optimization, Jacobian.
113 option      ~ 1
114
115 Restart by attempting to read breakpoint info
116

```

```

117 Note:    NO attempt was made to restart.
118
119 lmnt " 2, filename = air
120 lmnt " 5, filename = Si_02g
121 lmnt " 3, filename = Si
122
123 number of grid points scanned, kts =          4
124 population along the minimum, ktm =          1
125 norm of the residual, |g| = 1.17853E-04 (degrees)
126
127 model parameter value along the minimum:
128 1) 2.00014E+00, for: 2, (z)
129 2) 4.99959E-01, for: 5, (f)
130
131 -----
132 Statistics of deviations " experiment-model " g
133
134 where: g is a column vector of length 2M,
135        () denotes either (delta) or (psi)
136 mean () = m() = <g()> = (1/M) sum: g()
137 variance () = < (g() -m()) **2 >
138 covariance = < (g(1)-m(1))*(g(2)-m(2)) >
139 std dev = sqrt (variance)
140 correlat coef = covariance / (sd(1) * sd(2))
141
142          mean,      std dev      (degrees)
143 psi:      0.000      0.000
144 delta:    0.000      0.000
145          0.422 " correlation coefficient " <psi|delta>
146
147 [J(T)*J], renormalized for correlation.
148 1) 1.00000
149 2) 0.94674 1.00000
150
151 Normalization coefficients, sqrt: [J(T)*J]_(i,i)
152 2.90E-02 7.80E-02
153
154 rcond = 2.74E-02, condition number, [J(T)*J]
155
156 [J(T)*J]**(-1):
157 Determinant: 1.0369 E -1.0000
158 Inertia: ( 2 0 0), number of (+,-,0) eigenvalues.
159 Inverse: upper+diagonal matrix
160 1) 9.64E+00
161 2) -9.13E+00 9.64E+00
162
163 -----
164 The standard deviation of the residuals.
165
166 s(g) = sqrt [<gg>/(2M-N)] = 1.24228E-04 (degrees)
167
168
169 The estimated uncertainty in the model parameters,

```

```

170 assuming no correlation, i.e., diagonal terms only.
171
172          value,    uncertainty.
173      1)      2.0001      0.00023,    for:    2 " (z,zu)
174      2)      0.5000      0.00009,    for:    5 " (f,fu)
175
176 elapsed cpu-time = 52 centi-seconds
177                  + 0 seconds
178                  + 1 minutes

```

Regarding lines 173 and 174, one finds the values of the calculated uncertainty for the model parameters. Incidentally, it is also possible to calculate the uncertainty by inserting information from lines 132 to 168, i.e., "Statistics of deviations," into eq (24) directly, but then one must respect the mixed units of measure of the appropriate quantities. Regarding line 166, s_g is expressed in degrees. The Jacobian is expressed in radians and is scaled as well. To help one understand how the output data of the "Statistics of deviations" may be inserted into eq (24), consider as an example the calculation that yields the value of uncertainty shown on line 173. From eq (24), it follows that

$$\begin{aligned}
 \mathcal{U}(v_1) &= \left(\frac{\pi}{180} \right) s_g \left\{ \left[(\mathbf{J}_v^T \mathbf{J}_v)^{-1} \right]_{11} \right\}^{1/2} \\
 &\approx \left(\frac{3.14159}{180.0} \right) 1.24228 \times 10^{-4} \frac{\sqrt{9.64}}{2.9 \times 10^{-2}} \\
 &\approx 2.32 \times 10^{-4}
 \end{aligned}$$

where information has been taken from lines 166, 160, and 152.

The output file X.PLOT is given below.

```

1      1      msampl
2      1      mbien
3      1      1      mrpeat, imbien
4      10     2      mexpt, mu
5      1      1.50000E+00  7.00000E+01  0.00000E+00  1.70755E-05 (i,E,a, g (d,p))
6      2      2.00000E+00  7.00000E+01  2.73208E-05 -3.75660E-05 (i,E,a, g (d,p))
7      3      2.50000E+00  7.00000E+01  2.73208E-05 -7.51321E-05 (i,E,a, g (d,p))
8      4      3.00000E+00  7.00000E+01 -6.14717E-05 -2.04906E-05 (i,E,a, g (d,p))
9      5      3.50000E+00  7.00000E+01 -2.69547E-04 -5.12264E-05 (i,E,a, g (d,p))
10     6      4.00000E+00  7.00000E+01  3.62000E-04  3.07358E-05 (i,E,a, g (d,p))
11     7      4.50000E+00  7.00000E+01 -8.19623E-05 -1.16113E-04 (i,E,a, g (d,p))
12     8      5.00000E+00  7.00000E+01  5.46415E-05 -1.70755E-05 (i,E,a, g (d,p))
13     9      5.50000E+00  7.00000E+01 -1.36604E-04  1.70755E-05 (i,E,a, g (d,p))
14    10     6.00000E+00  7.00000E+01 -1.36604E-04 -4.09811E-05 (i,E,a, g (d,p))

```


5.4 Supplementary Parameters

As mentioned in the various subsections of section 4.2, supplementary parameters provide the user with additional degrees of freedom in characterizing the constituent and effective media. Currently, the program has incorporated only one constituent medium that requires a supplementary parameter, i.e., $\text{Al}_x\text{Ga}_{1-x}\text{As}$, where x refers to the aluminum mole fraction and ($0 \leq x \leq 0.8$). This may be seen by considering both the subroutine DIEL09 and its associated database file W.AL_GA_AS, see sections 6.5.9 and 6.6.7, respectively. The database contains profiles of the dielectric function as functions of energy for a set of discrete values (x_j) of the mole fraction of aluminum. To evaluate the dielectric function for intermediate values of x , subroutine DIEL09 linearly interpolates between two discrete profiles. Because of the rapid variations in the profiles and the coarseness of the (x_j) grid, a better approximation for $\epsilon(x)$ than that used here is possible by fitting the profiles of the dielectric functions with a set of oscillators as functions of the mole fraction (x). To provide this approximation, one would need to modify the subroutine DIEL09 appropriately. Incidentally, effects due to the internal electric field that is induced near the boundary between adjacent layers of GaAs and $\text{Al}_x\text{Ga}_{1-x}\text{As}$ where ($x > 0$) are not included here [6, 7].

The mechanism for making the proper correspondence between the model parameters and appropriate effective media and/or constituent media may be readily seen from the argument list of subroutines DIEFCN and DIELMN. The subroutine for the constituent medium receives supplementary parameters that are associated with the effective medium, as well as those associated with the ambient. Hence, it is incumbent on the subroutine of the constituent medium to interpret the information. Subroutine DIEL09 check-tests for the appropriate supplementary parameters, utilizes the parameters in calculating the constituent dielectric function, and calculates the appropriate partial derivative, which is required for any optimization variable. Regarding the supplementary parameters and their numerical values, the integer value labels the appropriate constituent medium, while the floating-point value provides the necessary relative concentration of aluminum.

For sake of demonstration, consider a room-temperature sample involving a substrate of GaAs and a top layer of $\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}$. Let the top layer thickness be 50 nm. Consider generating a set of measurement data for this structure. The input file X.DAT may be as follows.

```

1 drb1:[data_bases]w.
2 -----
3 1                      ! mfilmz / (j,z,zu,ivary)
4   1   50.   1.0   0    ! thickness, top layer
5 -----
6 1                      ! mipars / (i,ip)
7   1   9                ! lmnt " 9, constituent " AlGaAs
8 -----
9 1                      ! mrpars / (i,rp,up,ivary)
10  1   0.3   0.01   1    ! stoichiometry " x, Al(x)Ga(1-x)As
11 -----
12 3                      ! mixtures " number of effective media
13 1 0 0                  ! mlmnt,mipar,mrpar #1
14  1 2 1.0 0.0 0        ! j,lmnt,frac,ufrac,ivary " air
15 1 0 0                  ! mlmnt,mipar,mrpar #2
16  1 8 1.0 0.0 0        ! j,lmnt,frac,ufrac,ivary " GaAs
17 1 1 1                  ! mlmnt,mipar,mrpar #3
18  1 9 1.0 0.0 0        ! j,lmnt,frac,ufrac,ivary " AlGaAs
19  1 1                    ! i, iip
20  1 1                    ! i, irp
21 -----
22 1                      ! mbient " number of distinct ambients
23 1 1 0 0                ! j,imix,mipar,mrpar " air
24 -----
25 1                      ! msampl " number of samples
26 1                      ! mfilm " number of layers on sample #1
27 1 3 1                  ! j,imix,iz " AlGaAs
28 2 2                    ! j,imix " GaAs substrate
29 -----
30 1                      ! mbien " number of ambients for sample #1
31 1 1                    ! mrpeat,imbien
32  1                      ! mexpt " number of measurements
33  1   1.5   70.0   0.0   0.0   (i,E,a, d,p)
34   0.1   0.01   0.01   0.01   (uncertainty)

```

Again, the above last two lines involve pseudo measurement data.

Suppose now that measurement data are requested for energies that range between 1.5 and 4.0 eV with stepsize of 0.5 eV. Let the angles of incidence involve 65 and 70 deg. The input file X.INN may be as follows.

```

1 1                      ! forward problems, plots, ...
2 2                      ! grid scan
3 2                      ! (Delta, psi), x.dat
4 1.5 4.0 0.5           ! incident energy (eV)
5 65. 70. 5.0           ! incident angles (degrees)

```

The output file X.OUT is given below.

```

1  Enter:    sub-directory    for constituent media
2            sub-directory " drb1:[data_bases]w.
3
4  -----
5  Enter:    mfilmz " number of distinct widths
6            1            mfilmz " number of distinct widths
7  Enter:    i,z,zu,ivary
8            1    50.000    1.000    0    i,z,zu,ivary
9
10 -----
11 Enter:    mipars " number of parameters (integer)
12           1            mipars " number of parameters (integer)
13 Enter:    j, iparm    (# items= 1)
14           1            9    j, iparm
15
16 -----
17 Enter:    mrpars " number of parameters (floating-point)
18           1            mrpars " number of parameters (floating-point)
19 Enter:    j, rparm, uparm, ivary    (# items= 1)
20           1    3.00000E-01    1.00000E-02    1    (j,rparm,uparm,ivary)
21
22 -----
23 Enter:    mmixtr " number of distinct mixtures
24           3            mmixtr " number of distinct mixtures
25
26 Enter:    mlmnt, mipar, mrpar    (mix # 1)
27           1    0    0    mlmnt, mipar, mrpar
28 Enter:    j, lmnt, frac, ufrac, ivary
29           1    2    1.00000    0.00000    0    j, lmnt, frac, ufrac, ivary
30
31 Enter:    mlmnt, mipar, mrpar    (mix # 2)
32           1    0    0    mlmnt, mipar, mrpar
33 Enter:    j, lmnt, frac, ufrac, ivary
34           1    8    1.00000    0.00000    0    j, lmnt, frac, ufrac, ivary
35
36 Enter:    mlmnt, mipar, mrpar    (mix # 3)
37           1    1    1    mlmnt, mipar, mrpar
38 Enter:    j, lmnt, frac, ufrac, ivary
39           1    9    1.00000    0.00000    0    j, lmnt, frac, ufrac, ivary
40 Enter:    j, iiparm    (# items = 1)
41           1    1    j, iiparm
42 Enter:    j, irparm    (# items = 1)
43           1    1    j, irparm
44
45 -----
46 Enter:    mbient " number of distinct ambients
47           1            mbient " number of distinct ambients
48 Enter:    j, imix, mipar, mrpar
49           1    1    0    0    j, imix, mipar, mrpar
50
51 -----
52 Enter:    msampl " number of samples

```

```

53      1      msampl " number of samples
54
55 Enter:      mfilm " number of films on sample # 1
56      1      mfilm " number of films on sample # 1
57 Enter:      j, imix, iwidth      (film/substrate)
58      1      3      1      j, imix, iwidth
59      2      2      j, imix
60
61 -----
62 Enter:      mbien " number of ambients on sample # 1
63      1      mbien " number of ambients on sample # 1
64 Enter:      mrpeat, imbien
65      1      1      mrpeat, imbien
66 Enter:      mexpt " number of measurement data
67      1      mexpt " number of measurement data
68 Enter:      j, wavln (nm), angli,delta,psi (degree)
69      wavlnu      , anglu,deltu,psiu
70
71      1      1.500      70.000      0.000      0.000      (j, wavln,angli, delta,psi )
72      0.100      0.010      0.010      0.010      ( wavlu,anglu, deltu,psiu)
73
74
75 Enter:      option
76      1, forward problems, plots, ...
77      2, search      (vary)
78      3, search grid (vary)
79 option =      1
80
81
82 Enter:      choice of incident (energies, angles)
83      1, measurement data,      x.dat
84      2, grid scan.
85 choice =      2
86
87 Enter:      choice of output suitable for:
88      1, dielectric function, media,
89      2, (Delta, psi),      x.dat,
90      3, (Delta, psi),      plotting,
91      4, d/db,      b"(z,f,p),
92      5, d/da,      angle of incidence,
93      6, d/dE,      energy.
94 choice =      2
95
96 Enter:      range of incident energies (eV)
97 or:      - wavelengths (nm)
98 Enter:      ev1, ev2, ev3
99      1.5000      4.0000      0.5000      energy (eV)
100
101 Enter:      range of incident angles (degrees)
102 Enter:      angle1, angle2, angle3
103      65.0000      70.0000      5.0000      a1,a2,a3
104
105 lmnt " 2, filename = air

```



```

106  lmnt = 9,  filename = Al_Ga_As
107  lmnt = 8,  filename = Ga_As
108
109  elapsed cpu-time = 67  centi-seconds
110                   + 5  seconds

```

The requested measurement data of ellipsometric angles (Δ, ψ) are written to X.PLOT.
The output file X.PLOT is given below.

```

1      1      msampl
2      1      mbien
3      1      1      mrpeat, imbien
4      12      mexpt = measurements
5      1      1.50000E+00  6.50000E+01  1.76446E+02  1.24387E+01  (i,E,a, d,p)
6      1.00000E-01  1.00000E-02  1.00000E-02  1.00000E-02  (uncertainty)
7      2      2.00000E+00  6.50000E+01  1.79401E+02  1.57825E+01  (i,E,a, d,p)
8      1.00000E-01  1.00000E-02  1.00000E-02  1.00000E-02  (uncertainty)
9      3      2.50000E+00  6.50000E+01  1.77396E+02  1.95307E+01  (i,E,a, d,p)
10     1.00000E-01  1.00000E-02  1.00000E-02  1.00000E-02  (uncertainty)
11     4      3.00000E+00  6.50000E+01  1.66208E+02  2.33677E+01  (i,E,a, d,p)
12     1.00000E-01  1.00000E-02  1.00000E-02  1.00000E-02  (uncertainty)
13     5      3.50000E+00  6.50000E+01  1.49379E+02  2.43128E+01  (i,E,a, d,p)
14     1.00000E-01  1.00000E-02  1.00000E-02  1.00000E-02  (uncertainty)
15     6      4.00000E+00  6.50000E+01  1.48705E+02  2.35367E+01  (i,E,a, d,p)
16     1.00000E-01  1.00000E-02  1.00000E-02  1.00000E-02  (uncertainty)
17     7      1.50000E+00  7.00000E+01  1.69646E+02  4.65575E+00  (i,E,a, d,p)
18     1.00000E-01  1.00000E-02  1.00000E-02  1.00000E-02  (uncertainty)
19     8      2.00000E+00  7.00000E+01  1.78701E+02  8.31343E+00  (i,E,a, d,p)
20     1.00000E-01  1.00000E-02  1.00000E-02  1.00000E-02  (uncertainty)
21     9      2.50000E+00  7.00000E+01  1.75534E+02  1.26304E+01  (i,E,a, d,p)
22     1.00000E-01  1.00000E-02  1.00000E-02  1.00000E-02  (uncertainty)
23     10     3.00000E+00  7.00000E+01  1.58723E+02  1.75083E+01  (i,E,a, d,p)
24     1.00000E-01  1.00000E-02  1.00000E-02  1.00000E-02  (uncertainty)
25     11     3.50000E+00  7.00000E+01  1.35016E+02  1.96919E+01  (i,E,a, d,p)
26     1.00000E-01  1.00000E-02  1.00000E-02  1.00000E-02  (uncertainty)
27     12     4.00000E+00  7.00000E+01  1.33538E+02  1.88574E+01  (i,E,a, d,p)
28     1.00000E-01  1.00000E-02  1.00000E-02  1.00000E-02  (uncertainty)

```

6. Listing of Software Source Files and Routines

This section presents a listing of the source files for MAIN2. For convenience, the files are partitioned into six subsections. The first subsection involves files associated with storage arrays. The second subsection involves source programs that govern the direct or forward problem and the command options. The third subsection involves general utilities that provide basic tasks for the source programs. The fourth subsection involves source routines associated with evaluating the dielectric function for the effective media. The fifth subsection involves source routines associated with evaluating the dielectric function for the constituent media. The sixth subsection involves the databases that are associated with the constituent media.

For convenience, a brief orientation of the organization of the software development may be found in file A.HLP.

```
1  Notes:
2
3  1)  FORWRD solves the direct or forward problem.
4      The model parameters of sample include:
5          (z,e) " (thickness, dielectric function)
6      The dielectric function involves variables: (f,p)
7      FORWRD calculates: R, dR/dz, dR/de, dR/da.
8      Regarding (f,p), one needs: de/df, de/dp
9      so the Jacobian involves: J(z,f,p)
10     where: z " film thicknesses,
11            f " volume fractions of effective medium,
12            p " parameters local to constituents,
13            e " dielectric function,
14            a " angle of incidence
15
16  2)  EMA:      1 = sum(j): f(j),      j indexes constituent media.
17
18  3)  Organization of software development:
19
20     A)  Enter relevant information for processing.
21         1)  DEFNIT " define parameters controlling array allocation.
22         2)  MAIN   " main program " command processing of input data.
23         3)  INPDAT " input data to describe: models + measurements.
24
25     B)  Command options for simulation, plotting, etc.
26         1)  SCATOS " decision branch/tree
27         2)  SCATO1 " scan grid, domain input measurement data
28         3)  SCATO2 " scan grid, domain contiguous
29         4)  SCANO1 " scan grid of model parameters, evaluate |g|
30
31     C)  Minimize the residual in the least-squares sense.
```

```

32      1) SEEK01 - search:    single, unbounded
33      2) SEEK02 - used by:   SCAN02
34      3) SCAN02 - scan grid of (vary) model parameters
35
36      D) Construct the necessary sparse matrices,    b=Ax
37      1) ARRANG - construct pointers for sparse matrix - A
38      2) ASMBL - assemble the sparse matrices,    A,b
39      3) SCATTR - (psi,delta) for a single experiment.
40      4) FORWRD - (Rs, Rp, dRs, dRp) - direct or forward problem.
41      5) ASMBL0 - similar to the above, |g| only, no Jacobian.
42      6) SCATTO -
43      7) FORWRO -
44
45      E) Calculate the complex dielectric function, effective media.
46      1) DIEFCN - pass parameters to constituent media
47      2) DIEEMA - effective medium approximation
48      3) DIEMAD - calculate local partial derivatives
49      4) DIELMN - discern constituent media elements
50
51      F) Calculate the complex dielectric function, constituent media.
52      1) DIEL01 - vacuum
53      2) DIEL02 - air
54      3) DIEL03 - Silicon
55      4) DIEL04 - Silicon amorphous
56      5) DIEL05 - Silicon Dioxide (glass)
57      6) DIEL06 - Silicon Nitride (non-crystalline)
58      7) DIEL07 - Germanium
59      8) DIEL08 - Gallium Arsenide
60      9) DIEL09 - Aluminum Gallium Arsenide    (x - stoichiometry)
61      10) DIEL10 - Gallium Arsenide Oxides
62      11) DIEL11 - Arsenic amorphous
63      12) DIEL12 - GaP
64      13) DIEL13 - GaSb
65      14) DIEL14 - InAs
66      15) DIEL15 - InP
67      16) DIEL16 - InSb
68      17) DIEL17 - AlSb
69      18) DIEL18 -
70      19) DIEL19 -
71      20) DIEL20 -

```

6.1 Named COMMON and BLOCK DATA Statements

6.1.1 IOUNIT.

```
1      common / iounit / inn, iout, idat, isout, iplt, iscr
```


6.1.2 DEFINIT.

```

1 c      The configuration of each sample is:      (ambient/films/substrate).
2 c      each film      is characterized by:      widths, mixture.
3 c      each mixture is characterized by:
4 c      elements + volume fractions, parameters.
5 c      The configuration of each experiment/measurement is:
6 c      (psi,delta| wavelength, incident angle, ambient,sample).
7
8 c      Note:   the ambient mixture is NOT allowed to undergo variation.
9 c      This imposition is accounted within:   nrowssf.
10 c      Further, the constraint of:   1 = sum: f
11 c      has also been accounted within:   rowssf.
12
13 c      nsampl " number of distinct sample configurations, films/substrate.
14 c      nfilms " number of films layers allowed atop a substrate.
15 c      nparms " number of distinct parameters per mixture/ambient.
16 c      nlmnts " number of distinct elemental dielectric functions, e(w).
17 c      nbient " number of distinct ambients allowed atop a sample.
18 c      nwaves " number of wavelengths incident on sample.
19 c      nanglx " number of incident angles per wavelength.
20 c      nrpeat " number of repeats of an experiment.
21
22      parameter (nsampl= 6)
23      parameter (nfilms= 10)
24      parameter (nparms= 4)
25      parameter (nlmnts= 20)           ! see:   DIELMN
26      parameter (nbient= 1)
27      parameter (nwaves=100)
28      parameter (nanglx= 10)
29      parameter (nrpeat= 1)
30
31      parameter (nrows = nfilms*2+1)           !      (z,e),(e) "local
32                                           ! (z),(f,p),(p) "local
33      parameter (nrowssf= nfilms+(nfilms+1)*(nlmnts-1+nparms)+nparms)
34      parameter (nmixtr= nsampl*(nfilms+2))     ! mixtures "global
35      parameter (nfilmz= nsampl* nfilms)        ! z      "global
36      parameter (nrowss= nsampl*nrowssf+(nbient-1)*nparms) ! "global
37      parameter (nexpts= nsampl*nbient*nrpeat*nwaves*nanglx)
38      parameter (mrowss= nexpts*2)             ! (psi,delta)
39
40      complex   cmplx, conjg, sqrtt

```

6.1.3 FILMMM.

```

1      real    widths(nsampl*nfilms)      ! distinct widths of films
2      real    uwidth(nsampl*nfilms)      ! uncertainty in widths
3      integer lwidth(nsampl*nfilms)      ! variation    in widths
4
5      integer mmlmnt(nmixtr)              ! number of fractions per mixture
6      integer kklmnt(nmixtr)              ! offset location pointer
7      integer mvlmnt(nmixtr)              ! number of fractions varying in mix
8
9      integer iilmnt(nmixtr*nlmnts)       ! composition of mixture
10     real    fflmnt(nmixtr*nlmnts)       ! volume fraction
11     real    uflmnt(nmixtr*nlmnts)       ! uncertainty
12     integer lflmnt(nmixtr*nlmnts)       ! (vary/froz)
13
14     integer iiparm((nmixtr+nbient)*nparms) ! parameters
15     integer miparm( nmixtr+nbient)       ! number of parameters
16     integer kiparm( nmixtr+nbient)       ! offset
17     integer jiparm((nmixtr+nbient)*nparms) ! distribution
18
19     real    rrparm((nmixtr+nbient)*nparms) ! parameters
20     real    urparm((nmixtr+nbient)*nparms) ! uncertainty
21     integer lrparm((nmixtr+nbient)*nparms) ! (vary/froz)
22     integer mrparm( nmixtr+nbient)       ! number of parameters
23     integer mvparm( nmixtr+nbient)       ! number of parameters varying
24     integer krparm( nmixtr+nbient)       ! offset
25     integer jrparm((nmixtr+nbient)*nparms) ! distribution
26
27     integer mixmbn(nbient)                ! ambient
28
29     integer mmfilm(nsampl)                ! number of films on sample
30     integer kkfilm(nsampl)                ! offset
31     integer iifilm(nsampl*nrows)          ! (z,mixture),(mixture)
32
33     common / filmmm / widths, uwidth, lwidth, mfilmz,
34     &      mmlmnt, kklmnt, mvlmnt, nmixtr,
35     &      iilmnt, fflmnt, uflmnt, lflmnt, mlmnts,
36     &      iiparm, mipars,
37     &      rrparm, urparm, lrparm, mrpars,
38     &      miparm, kiparm, jiparm,
39     &      mrparm, mvparm, krparm, jrparm,
40     &      mixmbn, mbient,
41     &      mmfilm, kkfilm, iifilm, msampl

```

6.1.4 XPRMNT.

```
1      real  psiiis(nexpts), psiiiu(nexpts)
2      real  deltas(nexpts), deltau(nexpts)
3      real  angles(nexpts), angleu(nexpts)
4      real  wavlns(nexpts), wavlnu(nexpts)
5
6      integer mmbent(nsampl)
7      integer iibent(nsampl*nbient)
8      integer mmpeat(nsampl*nbient)
9      integer mmexpt(nsampl*nbient*nrpeat)
10
11     common / xprmnt / psiiis, psiiiu, deltas, deltau,
12     &          angles, angleu, wavlns, wavlnu,
13     &          mmbent, iibent, mmpeat, mmexpt, mexpts
```

6.1.5 FILMSS.

```
1 c      Each sample is characterized by the film/substrate:
2 c      geometry:    air / z(1) / ... / z(nfilms) / substrate
3 c      parameters:  three data (z,f,p) for each film,      may vary.
4 c                  two  data ( ,f,p) for the substrate, may vary.
5 c                  one  data ( ,f,p) for the air,   may not vary.
6
7 c      epsilon = electric permittivity ~ dielectric function ~ 1
8 c      sigma   = specific conductivity ~ 0
9 c      mu      = magnetic permeability ~ 1
10 c      omega   = angular frequency
11 c      die_r   = epsilon * mu
12 c      die_i   = 4*pi * sigma * mu / omega
13
14      complex die(nfilms+1)
15      real    zzz(nfilms ), air
16      integer mfilm
17
18      common / filmss / die, zzz, air, mfilm
```


6.1.6 ARRAYD.

```
1      integer  mixflm(nfilms+2)
2      logical  firstx(nmixtr)
3
4      complex  dielec(nmixtr)      ! (e) ~ dielectric function
5      complex  dielew(nmixtr)      ! d(e) /d (energy ~ eV)
6      complex  dielff(nlmnts,nmixtr) ! d(e) /d (volume fraction)
7      complex  dielpp(nparms,nmixtr) ! d(e) /d (parameter mixture)
8      complex  dielpa(nparms,nmixtr) ! d(e) /d (parameter ambient)
9
10     common / arrayd / dielec, dielew, dielff, dielpp, dielpa,
11     &          mixflm, firstx
```

6.1.7 ARRAYS.

```
1  c*    parameter (nnjaaa = mrowss*nrowss)          ! estimated need
2         parameter (nnjaaa = 2000000)              ! convenience
3
4         integer ja(nnjaaa), ia(mrowss+1)
5         real    aa(nnjaaa), bb(mrowss ), cc(mrowss)
6         real    xx(nrowss)
7
8         integer iptu(nrowss), iptv(nrowss), iptw(nrowss), iptx(nrowss)
9         logical llnorm
10
11        common / arrays / aa, bb, cc, xx, ja, ia,
12        &          iptu, iptv, iptw, iptx,
13        &          meqns, mvary, mfroz, llnorm
```

6.1.8 ABCDEF.

```
1      real      a(nrowsf*2), b(2), c(4)
2
3      common / abcdef / a,b,c
```

6.1.9 RSTACK.

```

1  c      Accessed or used by:   FORWRD, SCATTR
2
3  c      wavenumber = 2*pi/wavelength,      wavelength = nano-meters
4
5  c      d/dw (total derivative wrt frequency ) =
6  c      d/dq (partial derivative wrt wavenumber) * (dq/dw) +
7  c      d/de (partial wrt dielectric function) * (de/dw)
8
9      complex  Rs,      Rp      ! reflection coeff in ambient
10     complex  dRs(nrows), dRp(nrows) ! Jacobians
11     complex  dRsa,      dRpa    ! d/d(angle of incidence)
12     complex  dRsq,      dRpq    ! d/d(wavenumber)
13
14     common / rstack / Rs,Rp, dRs,dRp, dRsa,dRpa, dRsq,dRpq

```


6.1.10 WSTACK.

```
1      parameter (naat=(nrowss*(nrowss+1))/2)      ! upper triang + diag
2      real      aat (naat)                        ! A(T)*A
3      real      aats(nrowss)                      ! SCALJJ
4      integer   ipvt(nrowss)                      ! LINPACK workspace
5
6      real      p(mrowss), u(mrowss)              ! SCALII, CGN
7      real      v(nrowss), w(nrowss), xw(nrowss), se(nrowss)
8
9      common / wstack / aat,aats,ipvt,    p,u,  v,w,xw,se
```

6.1.11 ELMNTS.

```
1  c      Discern which among the files containing spectroscopic data
2  c      that describes the:  (dielectric functions, conductivities) (w),
3  c      have been accessed or otherwise opened.
4
5      character*40  subdir          ! sub-directory
6      logical      llmnts(nlmnts)
7
8      common / elmnts / llmnts, subdir
```

6.1.12 NESTO1.

```
1 c      Nest of do-loops associated with the multi-parameter grid scan.
2 c      Purpose:   SCAN02   passes arguments onto:   SEEK02
3
4      integer      iiii(nrowss), iii2(nrowss)
5      real         pppp(nrowss), ppp1(nrowss), ppp2(nrowss), ppp3(nrowss)
6      real         psav(nrowss)
7
8      common / nesto1 / pppp, ppp1, ppp2, ppp3, psav,
9      &               iiii,      iii2
```

6.1.13 HANDYY.

```
1  c      Convenient/handy set of data information.
2
3  c*     data      pi / 3.14159265E+00 /
4  c*     data      cccc / 2.99792458E+17 / ! speed of light, (nano-m/sec)
5  c*     data      wavlev / 1239.852056 / ! hc, (nano-meters)-(electron-volts)
6
7         real      pi, cccc, wavlev
8         common / handy / pi, cccc, wavlev
```

6.1.14 BLKDAT.FOR

```
1      block data blkdat
2
3      include 'iounit.'
4      include 'handyy.'
5
6      data inn,iout,idat,isout,iplt,iscr / 5,6,7,8,9,10 /
7
8      data      pi / 3.14159265E+00 /
9      data      cccc / 2.99792458E+17 / ! speed of light, (nano-m/sec)
10     data wavlev / 1239.852056 / ! (nano-meters)-(electron-volts)
11
12     end
13
```


6.2 Source Programs

6.2.1 MAIN.FOR

```
1      program main
2      include 'iounit.'
3
4      call fileop                ! open input data files
5      call inpdat                ! read input data
6      call arrang                ! set up pointers
7      it1 = istance (i)          ! CPU time (milli-sec)
8
9      write (iout,101)
10     read (inn,*,err=21,end=21) ichoic
11     write (iout,102)           ichoic
12
13     goto (1,2,3), ichoic
14     goto 22
15
16     1 call scatos                ! model ---> experiment
17         goto 11
18     2 call seeko1                ! single search for minimum
19         goto 11
20     3 call scano2                ! scan grid ( vary)
21         goto 11
22
23     11 it2 = istance (i)          ! CPU time (milli-sec)
24         it = (it2-it1)/10        ! CPU time (centi-sec) elapsed
25         its = 100                ! clock units / second
26         itm = its*60              ! / minute
27         ith = itm*60              ! / hour
28         itd = ith*24              ! / day
29
30         id = it/itd                ! days
31         it = it-id*itd
32         ih = it/ith                ! hours
33         it = it-ih*ith
34         im = it/itm                ! minutes
35         it = it-im*itm
36         is = it/its                ! seconds
37         it = it-is*its            ! remaining time in: centi-seconds
38
39     if (id.ne.0) then
40         write (iout,111) it, is, im, ih, id
41     else if (ih.ne.0) then
42         write (iout,111) it, is, im, ih
43     else if (im.ne.0) then
44         write (iout,111) it, is, im
45     else if (is.ne.0) then
46         write (iout,111) it, is
47     else
48         write (iout,111) it
```

```

49     end if
50
51     close (iout)
52     stop
53
54     21 write (iout,121)                ! error, opening file
55         stop
56     22 write (iout,122)                ! error, option choice
57         stop
58
59     101 format (/ ' Enter:  option      '
60         &      / 12x, '1,  forward problems, plots, ... '
61         &      / 12x, '2,  search      (vary)           '
62         &      / 12x, '3,  search grid (vary)           ' )
63     102 format ( ' option = ', i3 /)
64
65     111 format (/ ' elapsed cpu-time = ', i3, '  centi-seconds', :
66         &      /'                                + ', i3, '  seconds      ', :
67         &      /'                                + ', i3, '  minutes      ', :
68         &      /'                                + ', i3, '  hours        ', :
69         &      /'                                + ', i3, '  days          ' )
70
71     121 format (/ ' oops,  unable to access input data file  ' )
72     122 format (/ ' oops,  inconsistent with available options' )
73
74     end

```

6.2.2 FILEOP.FOR

```
1      subroutine fileop
2      include 'iounit.'
3
4
5      open ( inn,file='x.inn',status='old',readonly,shared)      ! 5
6      open ( idat,file='x.dat',status='old',readonly,shared)      ! 7
7
8      1 open ( iout,file='x.out',status='old',disp='delete',err=2) ! 6
9      close(iout)
10     goto 1
11     2 open ( iout,file='x.out',status='new')
12
13     3 open ( isout,file='x.sout',status='old',disp='delete',err=4) ! 8
14     close(isout)
15     goto 3
16     4 continue      ! open (isout,file='x.sout',status='new')
17
18     5 open ( iplt,file='x.plot',status='old',disp='delete',err=6) ! 9
19     close(iplt)
20     goto 5
21     6 open ( iplt,file='x.plot',status='new')
22
23     c* 7 open ( iscr,file='x.scr',status='old',disp='delete',err=8) ! 10
24     c* close(iscr)
25     c* goto 7
26     c* 8 continue      ! open (iscr,file='x.scr',status='new')
27
28     return
29     end
```

6.2.3 INPDAT.FOR

```

1      subroutine inpdatt
2      include 'iounitt.'
3      include 'defnitt.'
4      include 'filmmm.'
5      include 'xprmnt.'
6      include 'handyy.'          ! pi,cccc,wavlev
7      include 'elmnts.'          ! constituent media
8
9      logical   lvary             ! test whether something varies
10
11      raddeg = pi/180.0          ! radians/degree
12
13  c      =====
14  c      Sub-directory associated with database of constituent media.
15
16      write (iout,1001)
17      read  (idat,1002)  subdirt
18      write (iout,1003)  subdirt
19      write (iout,1004)
20      call ljchar (subdirt)      ! left-justify character string
21
22      do i=1,nlmnts
23          llmnts(i) = .false.    ! initialize
24      end do
25
26  c      =====
27  c      The dielectric function of each distinct element is
28  c      already available and provided via the subroutines.
29
30  c      Distinct widths
31
32      call hhline (idat,iout)    ! line of connected hyphens
33
34      write (iout,1011)
35      read  (idat,  *)  mfilmmz
36      write (iout,1012)  mfilmmz
37      if (mfilmmz.lt.0 .or. mfilmmz.gt.nfilmmz) then
38          write (iout,1013)
39          stop
40      end if
41      if (mfilmmz.ne.0) then
42          write (iout,1014)
43          do i=1,mfilmmz          ! distinct widths
44              read  (idat,  *)  j, z,zu, lvary
45              write (iout,1015) j, z,zu, lvary
46              if (j.ne.i .or.
47  &              z.lt.0.0 .or. zu.lt.0.0 .or.
48  &              lvary.lt.0 .or. lvary.gt.2 ) then
49                  write (iout,1016)
50                  stop

```

```

51         end if
52         if (ivary.eq.1 .and. zu.eq.0.0) then
53             write (iout,1017)
54             stop
55         end if
56         widths(i) = z
57         uwidth(i) = zu
58         lwidth(i) = ivary
59     end do
60 end if
61 write (iout,1004)
62 c =====
63 c Distinct supplementary parameters " integer
64
65 call hhline (idat,iout)          ! line of connected hyphens
66
67 write (iout,1021)
68 read (idat, *) mipars
69 write (iout,1022) mipars
70 if (mipars .lt. 0 .or.
71 &   mipars .gt. (nmixtr+nbient)*nparms) then
72     write (iout,1023)
73     stop
74 end if
75 if (mipars.ne.0) then
76     write (iout,1024) mipars
77     do i=1,mipars
78         read (idat, *) j, iparm
79         write (iout,1025) j, iparm
80         if (i.ne.j) then
81             write (iout,1026)
82             stop
83         end if
84         iiparm(i) = iparm
85     end do
86 end if          ! iiparm
87 write (iout,1004)
88 c =====
89 c Distinct supplementary parameters " floating-point
90
91 call hhline (idat,iout)          ! line of connected hyphens
92
93 write (iout,1031)
94 read (idat, *) mrpars
95 write (iout,1032) mrpars
96 if (mrpars .lt. 0 .or.
97 &   mrpars .gt. (nmixtr+nbient)*nparms) then
98     write (iout,1033)
99     stop
100 end if
101 if (mrpars.ne.0) then
102     write (iout,1034) mrpars
103     do i=1,mrpars

```



```

104         read (idat, *) j, rparm, uparm, ivary
105         write (iout,1035) j, rparm, uparm, ivary
106         if (i.ne.j .or. uparm.lt.0.0 .or.
107 &         ivary.lt.0 .or. ivary.gt.2 ) then
108             write (iout,1036)
109             stop
110         end if
111         if (ivary.eq.1 .and. uparm.eq.0.0) then
112             write (iout,1037)
113             stop
114         end if
115         rparm(i) = rparm
116         uparm(i) = uparm
117         lparm(i) = ivary
118     end do
119 end if ! rparm
120 write (iout,1004)
121 c =====
122 c Distinct effective media " mixtures
123
124 call hhline (idat,iout) ! line of connected hyphens
125
126 write (iout,1111)
127 read (idat, *) mmixtr ! number of distinct mixtures
128 write (iout,1112) mmixtr
129 write (iout,1004)
130 if (mmixtr.lt.1 .or. mmixtr.gt.nmixtr) then
131     write (iout,1113)
132     stop
133 end if
134 mlmnts = 0 ! total number of elements
135 kk = 0 ! index elements in the mixture
136 ki = 0
137 kr = 0
138 do m=1,mmixtr ! distinct mixtures
139     write (iout,1114) m
140     read (idat, *) mlmnt, mipar, mrpar
141     write (iout,1115) mlmnt, mipar, mrpar
142     if (mlmnt.lt.0 .or. mlmnt.gt.nlmnts .or.
143 &     mipar.lt.0 .or. mipar.gt.nparms .or.
144 &     mrpar.lt.0 .or. mrpar.gt.nparms .or.
145 &     (mlmnt+mrpar .eq. 0) ) then
146         write (iout,1116)
147         stop
148     end if
149 c -----
150     mv = 0 ! vary count
151     mmlmnt(m) = mlmnt ! number of elements in mixture
152     kklmnt(m) = kk ! offset
153     if (mlmnt.ne.0) then
154         mlmnts = mlmnts+mlmnt ! sum elements
155         sv = 0.0 ! vary
156         su = 0.0 ! froz

```

```

157       write (iout,1121)
158       do i=1,mlmnt                                ! composition
159         read (idat, *) j, lmnt, frac, ufrac, ivary
160         write (iout,1122) j, lmnt, frac, ufrac, ivary
161         if ( j.ne.i .or.
162           &      lmnt.lt.1 .or. lmnt.gt.nlmnts .or.
163           &      frac.lt.-0.5 .or. frac.gt.1.5 .or.
164           &      ufrac.lt.0.0 .or. ufrac.gt.1.0 .or.
165           &      ivary.lt.0 .or. ivary.gt.2 ) then
166           write (iout,1123)
167           stop
168         end if
169         if (ivary.eq.1 .and. ufrac.eq.0.0) then
170           write (iout,1124)
171           stop
172         end if
173         if (i.ne.1) then                                ! redundancy
174           do j=2,i
175             if (lmnt .eq. iilmnt(kk+2-j)) then
176               write (iout,1131)
177               stop
178             end if
179           end do
180         end if
181         kk = kk+1                                ! index
182         iilmnt(kk) = lmnt                        ! distinct element
183         fflmnt(kk) = frac                        ! volume fraction
184         uflmnt(kk) = ufrac                      ! uncertainty
185         lflmnt(kk) = ivary                      ! vary
186         if (lflmnt(kk).eq.1) then                ! vary
187           mv = mv+1
188           sv = sv+frac
189         else                                ! froz
190           su = su+frac
191         end if
192       end do                                ! elements
193
194       sum = sv+su                                ! vary+froz
195       if (sum.le.0.9 .or. sum.gt.1.1) then        ! consistency check
196         write (iout,1132)
197         stop
198       end if
199
200       if (mv.eq.0) then                                ! froz
201         if (abs(1.0-su) .gt. 1.0E-6) then        ! renormalize
202           write (iout,1133)
203           j = kk-mlmnt
204           do i=1,mlmnt
205             j = j+1
206             fflmnt(j) = fflmnt(j)/su            ! volume fraction
207           end do
208         end if
209       else if (mv.eq.1) then                    ! inconsistency

```

```

210         write (iout,1134)
211         stop
212     else                                     ! mv > 1
213         j = kk-mlmnt                         ! convenience
214         if (su .gt. 1.0) then                 ! consistency check
215             write (iout,1135)
216             stop
217         end if
218         if (sv .eq. 0.0) then                 ! renorm equally
219             write (iout,1136)
220             sv = (1.0-su)/float(mv)
221             do i=1,mlmnt
222                 j = j+1
223                 if (lflmnt(j).eq.1) then
224                     fflmnt(j) = sv           ! volume fraction
225                 end if
226             end do
227         else if (abs(1.0-sum) .gt. 1.0E-6) then ! renorm linearly
228             write (iout,1137)
229             v = (1.0-su)/sv                 ! vary(new)
230             do i=1,mlmnt
231                 j = j+1
232                 if (lflmnt(j).eq.1) then
233                     fflmnt(j) = v*fflmnt(j) ! volume fraction
234                 end if
235             end do
236         end if
237     end if                                     ! element test, vary+froz
238 end if                                     ! composition of elements
239 mvlmnt(m) = mv
240 c -----
241 miparm(m) = mipar                         ! number
242 kiparm(m) = ki                             ! offset
243 if (mipar.ne.0) then
244     write (iout,1141) mipar
245     do i=1,mipar
246         read (idat, *) j,ip                ! pointers
247         write (iout,1142) j,ip
248         if (j.ne.i .or. ip.lt.1 .or. ip.gt.mipars) then
249             write (iout,1143)
250             stop
251         end if
252         if (i.gt.1) then                    ! redundancy
253             do im=2,i
254                 if (ip .eq. jiparm(ki+2-im)) then
255                     write (iout,1144)
256                     stop
257                 end if
258             end do
259         end if
260         ki = ki+1
261         jiparm(ki) = ip                    ! distribution
262     end do

```

```

263         end if
264 c -----
265         mv = 0
266         mrparm(m) = mrpar                ! number
267         krparm(m) = kr                  ! offset
268         if (mrpar.ne.0) then
269             write (iout,1151) mrpar
270             do i=1,mrpar
271                 read (idat, *) j,ip                ! pointer
272                 write (iout,1152) j,ip
273                 if (j.ne.i .or. ip.lt.1 .or. ip.gt.mrpar) then
274                     write (iout,1153)
275                     stop
276                 end if
277                 if (i.gt.1) then                    ! redundancy
278                     do im=2,i
279                         if (ip .eq. jrparm(kr+2-im)) then
280                             write (iout,1154)
281                             stop
282                         end if
283                     end do
284                 end if
285                 kr = kr+1
286                 jrparm(kr) = ip                ! distribution
287                 if (lrparm(ip).eq.1) mv=mv+1
288             end do
289         end if
290         mvparm(m) = mv
291 c -----
292         write (iout,1004)
293     end do                ! mixtures
294 c =====
295 c Ambients & external parameters
296
297     call hhline (idat,iout)                ! line of connected hyphens
298
299     write (iout,1211)
300     read (idat, *) mbient
301     write (iout,1212) mbient
302     if (mbient.lt.1 .or. mbient.gt.nbient) then
303         write (iout,1213)
304         stop
305     end if
306     write (iout,1214)
307
308     do m=1,mbient
309         read (idat, *) j, imix, mipar, mrpar        ! additional
310         write (iout,1215) j, imix, mipar, mrpar      ! parameters
311         if ( j.ne.m .or.
312 &         imix.lt.1 .or. imix.gt.mmixtr .or.
313 &         mipar.lt.0 .or. mipar.gt.nparms .or.
314 &         mrpar.lt.0 .or. mrpar.gt.nparms ) then
315             write (iout,1216)

```

```

316         stop
317     end if
318
319     if (mvlmnt(imix).ne.0 .or. mvparm(imix).ne.0) then
320         write (iout,1217)
321         stop
322     end if
323
324     mixmbn(m) = imix      ! specify the mixture composing the ambient
325     mm = mmixtr+m        ! offset
326
327     miparm(mm) = mipar    ! number
328     kiparm(mm) = ki       ! offset
329     if (mipar.ne.0) then  ! parameters
330         write (iout,1221) mipar
331         do i=1,mipar
332             read (idat, *) j,ip      ! point to:  iiparm
333             write (iout,1222) j,ip
334             if (j.ne.i .or. ip.lt.1 .or. ip.gt.mipars) then
335                 write (iout,1223)
336                 stop
337             end if
338             if (i.ne.1) then          ! redundancy
339                 do j=2,i
340                     if (ip .eq. jiparm(ki+2-j)) then
341                         write (iout,1224)
342                         stop
343                     end if
344                 end do
345             end if
346             ki = ki+1
347             jiparm(ki) = ip          ! distribution
348         end do
349     end if
350
351     mv = 0
352     mrparm(mm) = mrpar    ! number
353     krparm(mm) = kr       ! offset
354     if (mrpar.ne.0) then  ! parameter
355         write (iout,1231) mrpar
356         do i=1,mrpar
357             read (idat, *) j,ip      ! point to:  rrparm
358             write (iout,1232) j,ip
359             if (j.ne.i .or. ip.lt.1 .or. ip.gt.mrpars) then
360                 write (iout,1233)
361                 stop
362             end if
363             if (i.ne.1) then          ! redundancy
364                 do j=2,i
365                     if (ip .eq. jrparm(kr+2-j)) then
366                         write (iout,1234)
367                         stop
368                     end if

```



```

369             end do
370         end if
371         kr = kr+1
372         jrparm(kr) = ip                ! distribution
373         if (lrparm(ip).eq.1) mv=mv+1
374     end do
375 end if
376 mvparm(mm) = mv
377
378 end do                ! ambients + external parameters
379 write (iout,1004)
380 c =====
381 c Construction of sample configuration "layered structure.
382
383 call hhlne (idat,iout)                ! line of connected hyphens
384
385 write (iout,1311)
386 read (idat, *) msampl
387 write (iout,1312) msampl
388 write (iout,1004)
389 if (msampl.lt.1 .or. msampl.gt.nsampl) then
390     write (iout,1313)
391     stop
392 end if
393
394 k = 0
395 do is=1,msampl                ! films/substrate
396     write (iout,1321) is
397     read (idat, *) mfilm
398     write (iout,1322) mfilm,is
399     if (mfilm.lt.0 .or. mfilm.gt.nfilms) then
400         write (iout,1323)
401         stop
402     end if
403     mmfilm(is) = mfilm
404     kkfilm(is) = k                ! offset
405     mfilms = mfilm+1                ! films,substrate
406     lvary = .false.                ! something should vary
407
408     write (iout,1331)
409     do m=1,mfilms
410         if (m.eq.mfilms) then
411             read (idat, *) j, imixtr
412             write (iout,1332) j, imixtr
413         else
414             read (idat, *) j, imixtr, iwidth
415             write (iout,1333) j, imixtr, iwidth
416             if (iwidth.lt.1 .or. iwidth.gt.mfilmz) then
417                 write (iout,1334)
418                 stop
419             end if
420             k = k+1
421             iifilm(k) = iwidth

```

```

422         lvary = lvary .or. (lwidth(iwidth).eq.1) ! test vary
423     end if
424     if (imixtr.lt.1 .or. imixtr.gt.mmixtr) then
425         write (iout,1335)
426         stop
427     end if
428     if (j.ne.m) then                                ! sequential indexing
429         write (iout,1336)
430         stop
431     end if
432     if (m.ne.1) then                                ! adjacency of mixtures
433         if (m.eq.mfilms) then
434             kback = k                                ! previous mixture
435         else
436             kback = k-1                              ! previous mixture
437         end if
438         if (imixtr .eq. iifilm(kback)) then
439             mv = mvlmnt(imixtr)+mvparm(imixtr)
440             if (mv .ne. 0) then
441                 write (iout,1337)
442                 stop
443             end if
444         end if
445     end if
446     k = k+1
447     iifilm(k) = imixtr
448     lvary = lvary .or. (mvlmnt(imixtr).ne.0)
449     & .or. (mvparm(imixtr).ne.0)
450 end do ! films
451
452 c*     if (.not.lvary) then                            ! something should vary, however
453 c*         write (iout,1338)                          ! in SCAT02 we allow (mv=0)
454 c*         stop                                          ! so as to discern:
455 c*     end if                                           ! d() /d(incident angle)
456
457     write (iout,1004)
458 end do ! sample
459 c=====
460 c Test compactness of domain variables.
461
462 c=====
463 c Measurement data of ellipsometric angles by instrumentation.
464
465 call hhline (idat,iout)                                ! line of connected hyphens
466
467 ias = 0                                                  ! ambient,sample
468 iras = 0                                                ! repeat,ambient,sample
469 i = 0                                                    ! expt,repeat,ambient,sample
470 ii = 0                                                  ! overflow
471 nextp = nwaves*nanglx                                  ! convenience
472 do is=1,msampl
473     write (iout,1411) is
474     read (idat, *) mbien                                ! number of ambients

```

```

475      write (iout,1412) mbien,is
476      if (mbien.lt.1 .or. mbien.gt.mbieent) then
477          write (iout,1413)
478          stop
479      end if
480      mmbent(is) = mbien                ! number of ambients
481      do mbn=1,mbien                  ! distinct ambients
482          write (iout,1421)
483          read (idat, *) mrpeat, imbien
484          write (iout,1422) mrpeat, imbien
485          if (mrpeat.lt.1 .or. mrpeat.gt.nrpeat .or.
486              &      imbien.lt.1 .or. imbien.gt.mbieent ) then
487              write (iout,1423)
488              stop
489          end if
490          if (mbn .ne. 1) then          ! redundancy
491              do j=2,mbn
492                  if (imbien .eq. iibent(ias+2-j)) then
493                      write (iout,1424)
494                      stop
495                  end if
496              end do
497          end if
498
499          ias = ias+1
500          iibent(ias) = imbien          ! specify ambient
501          mmpeat(ias) = mrpeat          ! number of repeats
502          do irpeat=1,mrpeat
503              write (iout,1431)
504              read (idat, *) mexpt
505              write (iout,1432) mexpt
506              if (mexpt.lt.1 .or. mexpt.gt.nexpt) then
507                  write (iout,1433) nexpt
508                  stop
509              end if
510              iras = iras+1
511              mmexpt(iras) = mexpt      ! number of experiments
512              write (iout,1441)
513              do ixpt=1,mexpt          ! (wave, incident angle)
514
515                  read (idat, *) j, wave, angl, delta, psi
516                  write (iout,1442) j, wave, angl, delta, psi
517                  read (idat, *) wavu, angu, delu, psiu
518                  write (iout,1443) wavu, angu, delu, psiu
519
520                  if (delta .lt. 0.0) then ! [0, 360)
521                      delta = delta + 360.0
522                  else if (delta .ge. 360.0) then
523                      delta = delta - 360.0
524                  end if
525
526  -----
527  c      The above measurement data is found from instrumentation.
528  c      Azzam and Horowitz assume:  n-ik ---> (Delta,psi) (Nebraska)

```

```

528 c      Here, we assume:  n+ik ---> (Delta,psi) (physics )
529 c      The convention affects only Delta.
530 c      The relationship is:  (physics) <--- conjg (Nebraska)
531
532          if (delta .ne. 0.0) then
533              delta = 360.0 - delta
534          end if
535 c      -----
536
537          if (wave .lt. 0.0) then                ! wavelength
538              if (wave .lt. -1240.0 .or.         ! nm
539                  & wave .gt. -200.0 .or.
540                  & wavu .le. 0.0 .or.
541                  & wavu .gt. 1000.0 ) then
542              write (iout,1444)
543              stop
544          end if
545 c*          wavu = -wavu/wave                    ! > 0
546 c*          wave = -wavlev/wave                 ! eV
547 c*          wavu = wave*wavu                   ! eV
548          else if (wave .lt. 1.0 .or.           ! energy
549                  & wave .gt. 6.0 .or.
550                  & wavu .lt. 0.0 .or.
551                  & wavu .gt. 6.0 ) then
552              write (iout,1444)
553              stop
554          end if
555
556          if (angl .lt.0.0 .or. angl .gt. 90.0 .or.
557              & angu .lt.0.0 .or. angu .gt. 1.0 .or.
558              & psi .lt.0.0 .or. psi .gt. 90.0 .or.
559              & psiu .lt.0.0 .or. psiu .gt.1000.0 .or.
560              & delta.lt.0.0 .or. delta.ge. 360.0 .or.
561              & delu .lt.0.0 .or. delu .gt.1000.0 ) then
562              write (iout,1444)
563              stop
564          end if
565
566          angu = amax1 (angu, 0.01) ! convenience
567          delu = amax1 (delu, 0.01)
568          psiu = amax1 (psiu, 0.01)
569
570          angl = angl *raddeg          ! radian <--- degree
571          angu = angu *raddeg
572          psi = psi *raddeg
573          psiu = psiu *raddeg
574          delta = delta*raddeg
575          delu = delu *raddeg
576
577          if (i.lt.nexpts) then
578              i = i+1
579              wavlms(i) = wave          ! -nm, +eV
580              wavlmu(i) = wavu

```

```

581             angles(i) = angl.           ! radians
582             angleu(i) = angu
583             psiiiis(i) = psi
584             psiiiu(i) = psiu
585             deltas(i) = delta
586             deltau(i) = delu
587             else                           ! overflow
588                 ii = ii+1
589             end if
590         end do           ! experiment, measurement
591         write (iout,1004)           ! blank line
592     end do           ! repeat
593 c -----
594         end do           ! ambient
595     end do           ! sample
596
597     if (ii.ne.0) then
598         i = i+ii
599         write (iout,1445) nexpts,i
600         stop
601     end if
602     mexpts = i           ! number of measured data
603
604     return
605
606 1001 format ( ' Enter:      sub-directory      for constituent media')
607 1002 format (a)
608 1003 format ( '              sub-directory " ', a)
609 1004 format ( ' ')
610
611 1011 format ( ' Enter:      mfilmz " number of distinct widths')
612 1012 format ( 1x, i4, 7x, 'mfilmz " number of distinct widths')
613 1013 format (/ ' ... oops, inconsistency')
614 1014 format ( ' Enter:      ',          24x, 'i,z,zu,ivary')
615 1015 format ( 1x, i4, 2f10.3, i5, 4x, 'i,z,zu,ivary')
616 1016 format (/ ' ... oops, inconsistency')
617 1017 format (/ ' ... oops, let:      zu > 0.0')
618
619 1021 format ( ' Enter:      mipars " number of parameters (integer)')
620 1022 format ( 1x, i4, 7x, 'mipars " number of parameters (integer)')
621 1023 format (/ ' ... oops, inconsistency')
622 1024 format ( ' Enter:      ',          13x, 'j, iparm      (# items=',i2,')')
623 1025 format ( 1x, i4, 4x, i10, 4x, 'j, iparm')
624 1026 format (/ ' ... oops, inconsistency')
625
626 1031 format ( ' Enter:      mrpars " number of parameters ',
627             &                               '(floating-point)')
628 1032 format ( 1x, i4, 7x, 'mrpars " number of parameters ',
629             &                               '(floating-point)')
630 1033 format (/ ' ... oops, inconsistency')
631 1034 format ( ' Enter:      j, rparm, uparm, ivary      (# items=',i2,')')
632 1035 format ( 1x, i4, 3x, 1p2e13.5, 4x, i1, 4x,
633             &                               '(j, rparm, uparm, ivary)' )

```



```

834 1036 format (/ ' ... oops, inconsistency')
835 1037 format (/ ' ... oops, let:      uparm /= 0.0 ')
836
837
838 1111 format ( ' Enter:      mmixtr ~ number of distinct mixtures')
839 1112 format ( 1x, i4, 7x, 'mmixtr ~ number of distinct mixtures')
840 1113 format (/ ' ... oops, inconsistency')
841 1114 format ( ' Enter:      mlmnt, mipar, mrpar      (mix #',i2,')')
842 1115 format ( 1x, 3i4, 3x,      'mlmnt, mipar, mrpar')
843 1116 format (/ ' ... oops, inconsistency')
844
845 1121 format ( ' Enter:      ', 30x, 'j, lmnt, frac, ufrac, ivary')
846 1122 format ( 1x, i4, i5, 2f10.5, i5, 5x,
847      &      'j, lmnt, frac, ufrac, ivary')
848 1123 format (/ ' ... oops, inconsistency')
849 1124 format (/ ' ... oops, let:      ufrac > 0.0')
850
851 1131 format (/ ' ... oops, redundancy among: lmnt')
852 1132 format (/ ' ... oops, sum of fractions not equal to unity')
853 1133 format (/ Note:      renormalizing frozen fractions,'
854      &      /'      since the mixture in the layer is frozen')
855 1134 format (/ ' ... oops, unable to vary one fraction, alone')
856 1135 format (/ ' ... oops, constraint upon: vary')
857 1136 format (/ Note:      renormalizing vary fractions, equally ')
858 1137 format (/ Note:      renormalizing vary fractions, linearly')
859
860 1141 format ( ' Enter:      ', 4x, 'j, iiparm      (# items =',i2,')')
861 1142 format ( 1x, i4, i5,      4x, 'j, iiparm')
862 1143 format (/ ' ... oops, inconsistency')
863 1144 format (/ ' ... oops, redundancy in: iiparm')
864
865 1151 format ( ' Enter:      ', 4x, 'j, irparm      (# items =',i2,')')
866 1152 format ( 1x, i4, i5,      4x, 'j, irparm')
867 1153 format (/ ' ... oops, inconsistency')
868 1154 format (/ ' ... oops, redundancy in: irparm')
869
870
871 1211 format ( ' Enter:      mbient ~ number of distinct ambients')
872 1212 format ( 1x, i4, 7x, 'mbient ~ number of distinct ambients')
873 1213 format (/ ' ... oops, inconsistency')
874 1214 format ( ' Enter:      ', 14x, 'j, imix, mipar, mrpar')
875 1215 format ( 1x, i4, 3i5,      4x, 'j, imix, mipar, mrpar')
876 1216 format (/ ' ... oops, inconsistency')
877 1217 format (/ ' ... oops, the ambient mixture should NOT vary,'
878      &      /'      but the ambient parameters may vary')
879
880 1221 format ( ' Enter:      ', 4x, 'j, iiparm      (# items=', i2, ')')
881 1222 format ( 1x, i4, i5,      4x, 'j, iiparm')
882 1223 format (/ ' ... oops, inconsistency')
883 1224 format (/ ' ... oops, redundancy ')
884
885 1231 format ( ' Enter:      ', 5x, 'j, irparm      (# items=', i2, ')')
886 1232 format ( 1x, i4, i5,      5x, 'j, irparm')

```

```

687 1233 format (/ ' ... oops, inconsistency')
688 1234 format (/ ' ... oops, redundancy ')
689
690
691 1311 format ( ' Enter:      msampl " number of samples')
692 1312 format ( 1x, i4, 7x, 'msampl " number of samples')
693 1313 format (/ ' ... oops, inconsistency')
694
695 1321 format ( ' Enter:      mfilm " number of films on sample #', i2)
696 1322 format ( 1x, i4, 7x, 'mfilm " number of films on sample #', i2)
697 1323 format (/ ' ... oops, inconsistency')
698
699 1331 format ( ' Enter:      ', 10x, 'j, imix, iwidth', 4x,
700      &                                '(film/substrate)')
701 1332 format ( 1x, i4, i5, 10x, 'j, imix ')
702 1333 format ( 1x, i4, 2i5, 5x, 'j, imix, iwidth')
703 1334 format (/ ' ... oops, inconsistency in: iwidth')
704 1335 format (/ ' ... oops, inconsistency in: imixtr')
705 1336 format (/ ' ... oops, inconsistency in: j ')
706 1337 format (/ ' ... oops, two adjacent mixtures are identical,
707      &      /' yet undergoing variation. Why ? ')
708 1338 format (/ ' ... oops, inconsistency " nothing is varying'
709      &      /' neither width nor mixture parameter')
710
711
712 1411 format ( ' Enter:      mbien " number of ambients on sample #',
713      &                                i2)
714 1412 format ( 1x, i4, 7x, 'mbien " number of ambients on sample #',
715      &                                i2)
716 1413 format (/ ' ... oops, inconsistency')
717
718 1421 format ( ' Enter:      ', 4x, 'mrpeat, imbien')
719 1422 format ( 1x, i4, i5, 4x, 'mrpeat, imbien')
720 1423 format (/ ' ... oops, inconsistency')
721 1424 format (/ ' ... oops, redundancy ')
722
723 1431 format ( ' Enter:      mexpt " number of measurement data')
724 1432 format ( 1x, i4, 7x, 'mexpt " number of measurement data')
725 1433 format (/ ' ... oops, inconsistency, nwaves*nanglx=', i5)
726
727 1441 format ( ' Enter:      j, wavln (nm), angli,delta,psi (degree)'
728      &      /' wavlnu , anglu,deltu,psiu ')
729 1442 format ( 1x, i4, f10.3, f10.3, f10.3, f10.3,
730      &      5x, '(j, wavln,angli, delta,psi )')
731 1443 format ( 5x, f10.3, f10.3, f10.3, f10.3,
732      &      5x, '( wavlu,anglu, deltu,psiu)')
733 1444 format (/ ' ... oops, inconsistency')
734 1445 format (/ ' ... oops, increase the value of: nexpts'
735      &      /' from:', i5, ', to:', i5)
736
737      end

```

6.2.4 SCATOS.FOR

```

1      subroutine scatoss                                ! simulate measurement data
2      include 'iounit.'
3      integer choice
4
5
6      write (iout,101)                                ! measurements vs. grid scan
7      read ( inn, *) choice                            ! involving source variables:
8      write (iout,102) choice                          ! photon energy, and
9      if (choice.lt.1 .or.                             ! angle of incidence
10     & choice.gt.2 ) then
11         write (iout,103)
12         stop
13     end if
14
15     if (choice.eq.1) then                            ! measurements: (E,a)
16         write (iout,111)
17         read ( inn, *) choice
18         write (iout,112) choice
19         if (choice.ge.1 .and.
20     & choice.le.3 ) then
21             call scatol (choice)
22         else if (choice.eq.4) then
23             call scanol
24         else
25             write (iout,113)
26             stop
27         end if
28
29     else if (choice.eq.2) then                        ! grid scan: (E,a)
30         write (iout,121)
31         read ( inn, *) choice
32         write (iout,122) choice
33         if (choice.lt.1 .or.
34     & choice.gt.6 ) then
35             write (iout,123)
36             stop
37         end if
38         call scato2 (choice)
39     end if
40
41     return
42
43 101 format (/ ' Enter: choice of incident (energies, angles)'
44     & / 12x, '1, measurement data, x.dat'
45     & / 12x, '2, grid scan. ')
46 102 format ( ' choice = ', i3)
47 103 format (/ ' scatoss, ... oops, inconsistent choice')
48
49 111 format (/ ' Enter: choice of output suitable for: '
50     & / 12x, '1, input data, x.dat, ')

```

```

51      &      / 12x, '2,   plotting (Delta, psi),
52      &      / 12x, '3,   plotting (Delta, psi) deviations,'
53      &      / 12x, '    deviation = measurement - model,'
54      &      / 12x, '4,   plotting |g| " rms deviation, unscaled,'
55      &      / 12x, '    on a 1D or 2D grid of model parameters.')
56 112 format ( ' choice = ', i3)
57 113 format (/ ' scatos, ... oops, inconsistent choice')
58
59 121 format (/ ' Enter:  choice of output suitable for: '
60      &      / 12x, '1,   dielectric function,  media,'
61      &      / 12x, '2,   (Delta, psi),          x.dat,'
62      &      / 12x, '3,   (Delta, psi),          plotting,'
63      &      / 12x, '4,   d/db,                  b"(z,f,p),'
64      &      / 12x, '5,   d/da,          angle of incidence,'
65      &      / 12x, '6,   d/dE,          energy.')
66 122 format ( ' choice = ', i3)
67 123 format (/ ' scatos, ... oops, inconsistent choice')
68
69      end

```

6.2.5 SCATOLFOR

```

1  c  -----
2  c  Input the range parameters for the grid scan, (energy, angle)
3  c  -----
4
5      subroutine scatol (mevs, ev1, ev2, ev3,
6      &                  mang, ang1, ang2, ang3 )
7      include 'iounit.'
8      include 'handyy.'                      ! pi,cccc,wavlev
9
10 c  -----
11 c  Optical frequency, wavelength, or associated photon energy.
12 c  -----
13
14      write (iout,111)                      ! incident energy
15      read  ( inn, *) ev1, ev2, ev3          ! -nm, +eV
16
17      if (ev1.lt.0.0 .and. ev2.gt.0.0 .or.    ! no mixing
18      &    ev1.gt.0.0 .and. ev2.lt.0.0 .or.
19      &    ev1.gt.ev2                          ) then
20          write (iout,114)
21          stop
22      end if
23
24      if (ev1 .lt. 0.0) then
25          write (iout,112) ev1, ev2, ev3      ! -nm, wavelength
26          if (ev1 .eq. ev2) then
27              m = 1                          ! number of steps
28          else if (ev3 .eq. 0.0) then
29              m = 2
30          else
31              m = max (1, nint (abs ( (ev2-ev1)/ev3 )))
32          end if
33          ev1 = -wavlev/ev1                    ! +eV, energy
34          ev2 = -wavlev/ev2
35          ev3 = (ev2-ev1)/float (max (1, m-1))
36      end if
37      write (iout,113) ev1, ev2, ev3
38
39      if (ev1.lt.1.0 .or. ev2.gt.6.0 .or.      ! Check-test
40      &    ev3.lt.0.0 .or. ev2.lt.ev1          ) then
41          write (iout,114)
42          stop
43      end if
44
45      if (ev1.eq.ev2) then
46          mevs = 1
47          ev3 = 0.0
48      else if (ev3.eq.0.0) then
49          mevs = 2
50          ev3 = ev2-ev1

```



```

51     else
52         ev4 = ev2-ev1
53         mevs = 1 + nint (ev4/ev3)
54         if (mevs.eq.1) then
55             ev3 = ev4
56         else
57             ev3 = ev4/float (mevs-1)
58         end if
59     end if
60
61 c -----
62 c Angle of incidence
63 c -----
64
65     write (iout,121)                                ! incident angles
66     read ( inn, *)  ang1, ang2, ang3                 ! degrees
67     write (iout,122)  ang1, ang2, ang3
68     if (ang1.lt.0.0 .or. ang2.gt.90.0 .or.
69 &    ang3.lt.0.0 .or. ang2.lt.ang1    ) then
70         write (iout,123)
71         stop
72     end if
73
74     if (ang1.eq.ang2) then
75         mang = 1
76         ang3 = 0.0
77     else if (ang3.eq.0.0) then
78         mang = 2
79         ang3 = ang2-ang1
80     else
81         ang4 = ang2-ang1
82         mang = 1 + nint (ang4/ang3)
83         if (mang.eq.1) then
84             ang3 = ang4
85         else
86             ang3 = ang4/float (mang-1)
87         end if
88     end if
89 c -----
90     write (iout,131)
91
92     return
93
94     111 format (/ ' Enter:      range of incident energies (eV)'
95 &           /'      or:          - wavelengths (nm)'
96 &           /' Enter:      ev1, ev2, ev3      ')
97     112 format ( 1x, 3f10.2, 10x, 'wavelength (nm)' )
98     113 format ( 1x, 3f10.4, 10x, '  energy (eV)' )
99     114 format ( ' ... oops, inconsistent' )
100
101     121 format (/ ' Enter:      range of incident angles (degrees) '
102 &           /' Enter:      angle1, angle2, angle3      ')
103     122 format ( 1x, 3f10.4, 10x, 'a1,a2,a3' )

```

```
104 123 format ( ' ... oops, inconsistent')
105
106 131 format ( ' ')
107
108     end
```

6.2.6 SCATO1.FOR

```

1      subroutine scato1 (icase)
2
3      c -----
4      c Retain and use information specifying the configuration of the:
5      c 1) source probe " (angle of incidence, wavelength)
6      c 2) sample geometry " (z,f,p)
7
8      c Calculate the forward scattering problem " (Delta, psi).
9      c Simulate ellipsometric measurements of (Delta, psi).
10     c Format the output scattering data (Delta, psi):
11     c 1) suitable for INPDAT
12     c 2) suitable for plotting
13     c 3) suitable for plotting differences in the fit.
14     c difference = experiment - model
15
16     c The template for this routine is from: ASMBL
17     c -----
18
19     include 'iounit.'
20     include 'defnit.'
21     include 'filmm.'
22     include 'xprmnt.'
23     include 'arrayd.'
24     include 'arrays.'
25     include 'filmss.'
26     include 'abcdef.'
27     include 'handyy.' ! pi
28
29     logical first, firstv
30
31
32     raddeg = 180.0/pi
33
34     mmm = mfilmz+mlmnts+mrpars
35     do m=1,mmm ! local, column in a row of: aa
36         if (iptw(m).ne.-1) then ! utilized
37             iptw(m) = 0 ! global ---> local into: aa
38         end if
39         iptx(m) = 0 ! local ---> global into: iptw
40     end do
41
42     ize = 0 ! (z,e), sample
43     ias = 0 ! ambient, sample
44     iras = 0 ! repeat, ambient, sample
45     ixpts = 0 ! expt, repeat, ambient, sample
46
47     write (iplt,101) msampl
48
49     do is=1,msampl
50         mfilm = mmfilm(is) ! FILMSS

```

```

51      mfilms = mfilm+1                                !      films/substrate
52      mfilma = mfilm+2                                !      ambient/films/substrate
53      mzs = mfilm*2+1                                  !      (z,e),(e)
54      mv = 0                                            !      local, unique, vary
55
56      do m=1,mfilms
57          if (m.ne.mfilms) then                        !      films
58              ize = ize+1                              !      widths
59              iwidth = iifilm(ize)
60              zzz(m) = widths(iwidth)                  !      FILMSS
61              if (lwidth(iwidth).eq.1) then            !      vary
62                  j = iwidth
63                  if (iptw(j).eq.0) then                !      unique, compress
64                      mv = mv+1                          !      local
65                      iptw(j) = mv
66                      iptx(mv) = j
67                  end if
68              end if
69          end if
70          ize = ize+1                                    !      films/substrate
71          imixtr = iifilm(ize)                          !      mixture
72
73          mixflm(m) = imixtr                            !      initialize
74
75          mvlmn = mvlmnt(imixtr)                        !      vary
76          if (mvlmn.ne.0) then                          !      fraction
77              first = .true.                            !      constraint, 1=u+v
78              mmlmn = mmlmnt(imixtr)                    !      quantity
79              kk = kklmnt(imixtr)                       !      offset
80              do lmn=1,mmlmn
81                  kk = kk+1                              !      monotonic
82                  if (lflmnt(kk).eq.1) then              !      vary
83                      j = mfilmz+kk                      !      global
84                      if (first) then                    !      constraint on: dv(1)
85                          first = .false.
86                      else if (iptw(j).eq.0) then
87                          mv = mv+1                      !      local unique
88                          iptw(j) = mv
89                          iptx(mv) = j
90                      end if
91                  end if                                !      vary
92              end do                                    !      fraction
93          end if                                        !      something varies
94
95          mvpar = mvparm(imixtr)                        !      vary
96          if (mvpar.ne.0) then                          !      parameter
97              mrpar = mrparm(imixtr)                    !      quantity
98              kr = krparm(imixtr)                       !      offset
99              do irp=1,mrpar
100                  kr = kr+1                              !      offset
101                  ip = jrparm(kr)                       !      specify index
102                  if (lrparm(ip).eq.1) then              !      vary
103                      j = mfilmz+mmlmnts+ip             !      global, unique

```

```

104             if (iptw(j).eq.0) then !      unique
105                 mv = mv+1           !      local, compress, aa
106                 iptw(j ) = mv
107                 iptx(mv) = j
108             end if
109         end if      ! vary
110     end do          ! parameters
111 end if              ! something varies
112 end do              ! mfilms
113
114 mvsav = mv          ! convenience
115 mbien = mmhent(is)  ! quantity
116
117 write (iplt,102) mbien
118
119 do mbn=1,mbien      ! ambients
120     ias = ias+1
121     mrpeat = mmpeat(ias)
122     imbien = iibent(ias)      ! specify ambient
123     imixtr = mixmbn(imbien)   ! mixture used as ambient
124
125     mixflm(mfilms+1) = imixtr
126     mv = mvsav
127
128     write (iplt,103) mrpeat, imbien
129
130     mvlmn = mvlmnt(imixtr)    ! vary
131     if (mvlmn.ne.0) then      !      fractions
132         first = .true.
133         mmlmn = mmlmnt(imixtr)
134         kk = kklmnt(imixtr)   !      offset
135         do lmn=1,mmlmn        !      fractions
136             kk = kk+1
137             if (lflmnt(kk).eq.1) then !      vary
138                 j = mfilmz+kk
139                 if (first) then      !      constraint
140                     first = .false.
141                 else if (iptw(j).eq.0) then
142                     mv = mv+1        !      local, compress
143                     iptw(j ) = mv
144                     iptx(mv) = j
145                 end if
146             end if      ! vary
147         end do          ! fractions
148     end if              ! something varies
149
150     mvpar = mvparm(imixtr)    ! vary
151     if (mvpar.ne.0) then      !      parameters
152         mrpar = mrparm(imixtr)
153         kr = krparm(imixtr)   !      offset
154         do irp=1,mrpar
155             kr = kr+1
156             ip = jrparm(kr)    !      specify index

```



```

157         if (lrparm(ip).eq.1) then
158             j = mfilmz+mlmnts+ip
159             if (iptw(j).eq.0) then ! unique
160                 mv = mv+1
161                 iptw(j) = mv
162                 iptx(mv) = j
163             end if
164         end if
165     end do
166 end if
167
168 mm = mmixtr+imbien ! offset, ambient
169 mvpar = mvparm(mm) ! vary
170 if (mvpar.ne.0) then ! parameter
171     mrpar = mrparm(mm) ! quantity
172     kr = krparm(mm) ! offset
173     do irp=1,mrpar
174         kr = kr+1 ! offset
175         ip = jrparm(kr) ! specify index
176         if (lrparm(ip).eq.1) then ! vary
177             j = mfilmz+mlmnts+ip ! global
178             if (iptw(j).eq.0) then ! unique
179                 mv = mv+1 ! local, compress, aa
180                 iptw(j) = mv
181                 iptx(mv) = j
182             end if
183         end if
184     end do
185 end if ! something varies
186
187 mvari = mv ! local quantity
188 firstv = .true. ! yet need row: delta
189
190 do irpeat=1,mrpeat ! repeats
191     iras = iras+1
192     mexpt = mmexpt(iras)
193     m = 2
194     write (iplt,104) mexpt, m ! nx,nu /(i,x,u)
195
196     do ixpt=1,mexpt ! measurements
197         ixpts = ixpts+1
198
199         wavln1 = wavlns(ixpts) ! -nm, +eV
200         wavln2 = wavlnu(ixpts)
201         angle1 = angles(ixpts) ! radians
202         angle2 = angleu(ixpts)
203         psi1 = psiis(ixpts) ! radians
204         psi2 = psiiu(ixpts)
205         delta1 = deltas(ixpts) ! radians
206         delta2 = deltau(ixpts)
207
208         do m=1,mfilma ! initialize, indicate
209             i = mixflm(m)

```

```

210         firstx(i) = .true.      !    need of evaluation
211     end do
212
213 c       Discern:    dielectric functions (z)
214
215         imixtr = mixmbn(imbien)      ! ambient
216         firstx(imixtr) = .false.
217         call diefcfn (imbien, imixtr, angle1, wavln1,
218 &             dielec( imixtr), dielew( imixtr),
219 &             dielff(1,imixtr),
220 &             dielpp(1,imixtr), dielpa(1,imixtr))
221
222         ize = ize-mzs                ! reset pointer
223     do m=1,mfilms
224         if (m.ne.mfilms) then        ! skip widths
225             ize = ize+1
226         end if
227         ize = ize+1
228         imixtr = iifilm(ize)
229         if (firstx(imixtr)) then      ! first
230             firstx(imixtr) = .false.
231             call diefcfn (imbien, imixtr,
232 &                 angle1, wavln1,
233 &                 dielec( imixtr), dielew( imixtr),
234 &                 dielff(1,imixtr),
235 &                 dielpp(1,imixtr), dielpa(1,imixtr))
236         end if
237         die(m) = dielec(imixtr)
238     end do        ! films
239
240     isampl = is
241     izsmpl = ize-mzs                ! reset index
242     call scattnr (wavln1, angle1,
243 &         isampl, izsmpl, imbien, mvari)
244
245     angl = angle1*raddeg            ! degrees
246     psi  = b(1) *raddeg
247     delta = b(2) *raddeg
248     au   = angle2*raddeg
249     pu   = psi2 *raddeg
250     du   = delta2*raddeg
251
252     if (delta.lt.0.0) then           ! [0,360)
253         delta = delta + 360.0
254     end if
255     if (delta.ne.0.0) then           ! phase shift
256         delta = 360.0 - delta
257     end if
258
259 c -----
260 c       Now, consider the distinct formats for output
261
262     if (icase .eq. 1) then          ! for IMPDAT

```

```

283         write (iplt,105) ixpt, wavln1,angl,delta,psi
284         write (iplt,106)         wavln2, au, du, pu
285
286     else if (icase .eq. 2) then          ! for plotting
287         write (iplt,105) ixpt, wavln1,angl,delta,psi
288
289     else if (icase .eq. 3) then          ! diff = expt-model
290         dpsi = ( psi1-b(1)) *raddeg      ! degrees
291     c*         ddel = (delta1-b(2)) *raddeg
292         call differ (delta1, b(2), diff)! deviation, mod fcn
293         ddel = diff *raddeg
294         write (iplt,107) ixpt, wavln1,angl,ddel,dpsi
295     else                                  ! oops
296         call exit (2)
297     end if
298 c     -----
299     end do          ! measurements
300 end do              ! repeats
301
302     if (mv.gt.mvsav) then      ! reset unique-ness
303         mv1 = mvsav+1
304         do i=mv1,mv
305             j = iptx(i)        ! point to: iptw
306             iptw(j) = 0        ! unique-ness
307             iptx(i) = 0
308         end do
309     end if
310 end do              ! ambients
311
312     if (mvsav.ne.0) then      ! reset unique-ness
313         do i=1,mvsav
314             j = iptx(i)        ! point to: iptw
315             iptw(j) = 0        ! unique-ness
316             iptx(i) = 0
317         end do
318     end if
319 end do              ! sample
320
321     return
322
323 101 format (1x, i5,          15x,      'msampl')
324 102 format (1x, i5,          15x,      'mbien ')
325 103 format (1x, 2i5,         10x,      'mrpeat, imbien')
326 104 format (1x, 2i5,         10x,      'mexpt, mu')
327 105 format (1x, i5, 2x, 1p4e13.5, 2x, '(i,E,a, d,p) ')
328 106 format (          8x, 1p4e13.5, 2x, '(uncertainty)')
329 107 format (1x, i5, 2x, 1p4e13.5, 2x, '(i,E,a, g (d,p))')
330
331     end

```

6.2.7 SCATO2.FOR

```

1      subroutine scato2 (choice)                                ! grid scan, contiguous
2
3      c -----
4      c Perform a grid scan:      (wavelength-energy, incident angle)
5      c Output:      function:      dielectric function (energy), media
6      c               function:      (Delta, psi), uncertainties, x.dat
7      c               function:      (Delta, psi)
8      c               Jacobian:      (d/dz, d/df, d/dp)_(Delta, psi)
9      c               Jacobian:      (d/da      )_(Delta, psi)
10     c               Jacobian:      (d/dE      )_(Delta, psi)
11     c The template for this routine is from:  ASMBL
12     c -----
13
14     include 'iounit.'
15     include 'defnit.'
16     include 'filmmm.'
17     include 'xprmnt.'
18     include 'arrayd.'
19     include 'arrays.'
20     include 'filmss.'
21     include 'abcdef.'
22     include 'handyy.'                                ! pi,cccc,wavlev
23
24     logical  first, firstv
25     integer  choice
26
27
28     if (choice.eq.1) then                                ! dielectric function
29         write (iout,141)                                ! specify mixture
30         read  ( inn, *) kmix                             ! for plotting
31         write (iout,142) kmix
32         if (kmix.lt.1 .or. kmix.gt.mmixtr) then
33             write (iout,143)
34             stop
35         end if
36     end if
37
38     c Discern the bounds or domain of the grid.
39
40     call scatoi (mevs,  ev1,  ev2,  ev3,                ! wavelength-energy
41     &           mang, ang1, ang2, ang3 )                ! angles of incidence
42
43     c -----
44     mmm = mfilmm+mmlmnts+mrpars
45     do m=1,mmm                                           ! local, column in a row of:  aa
46         if (iptw(m).ne.-1) then                          ! utilized
47             iptw(m) = 0                                  ! global ---> local    into:  aa
48         end if
49         iptx(m) = 0                                       ! local ---> global    into:  iptw
50     end do

```

```

51
52 raddeg = 180.0/pi
53 ize = 0 ! (z,e) ,sample
54 ias = 0 ! ambient,sample
55 iras = 0 ! repeat,ambient,sample
56 ixpts = 0 ! expt,repeat,ambient,sample
57
58 write (iplt,211) msampl
59
60 do is=1,msampl
61   mfilm = mmfilm(is) ! FILMSS
62   mfilms = mfilm+1 ! films/substrate
63   mfilma = mfilm+2 ! ambient/films/substrate
64   mzs = mfilm*2+1 ! (z,e),(e)
65   mv = 0 ! local, unique, vary
66
67   if (choice.eq.1) then ! initialize
68     kmix = iabs (kmix) ! referencing
69   end if
70
71   do m=1,mfilms
72     if (m.ne.mfilms) then ! films
73       ize = ize+1 ! widths
74       iwidth = iifilm(ize)
75       zzz(m) = widths(iwidth) ! FILMSS
76       if (lwidth(iwidth).eq.1) then ! vary
77         j = iwidth
78         if (iptw(j).eq.0) then ! unique, compress
79           mv = mv+1 ! local
80           iptw(j) = mv
81           iptx(mv) = j
82         end if
83       end if
84     end if
85     ize = ize+1 ! films/substrate
86     imixtr = iifilm(ize) ! mixture
87     mixflm(m) = imixtr ! initialize
88
89     if (choice.eq.1) then
90       if (kmix.eq.imixtr) then ! referenced
91         kmix = -kmix ! negative
92       end if
93     end if
94
95     mvlmn = mvlmnt(imixtr) ! vary
96     if (mvlmn.ne.0) then ! fraction
97       first = .true. ! constraint, 1=u+v
98       mmlmn = mmlmnt(imixtr) ! quantity
99       kk = kklmnt(imixtr) ! offset
100      do lmn=1,mmlmn
101        kk = kk+1 ! monotonic
102        if (lflmnt(kk).eq.1) then ! vary
103          j = mfilmz+kk ! global

```



```

104         if (first) then          !      constraint, dv(1)
105             first = .false.
106         else if (iptw(j).eq.0) then
107             mv = mv+1              !      local unique
108             iptw(j) = mv
109             iptx(mv) = j
110         end if
111     end if          ! vary
112 end do             ! fraction
113 end if             ! something varies
114
115 mvpar = mvparm(imixtr)          ! vary
116 if (mvpar.ne.0) then            !      parameter
117     mrpar = mrparm(imixtr)      !      quantity
118     kr     = krparm(imixtr)     !      offset
119     do irp=1,mrpar
120         kr = kr+1                !      offset
121         ip = jrparm(kr)          !      specify index
122         if (lrparm(ip).eq.1) then !      vary
123             j = mfilmz+mlmnts+ip !      global, unique
124             if (iptw(j).eq.0) then !      unique
125                 mv = mv+1        !      local, compress, aa
126                 iptw(j) = mv
127                 iptx(mv) = j
128             end if
129         end if          ! vary
130     end do              ! parameters
131 end if                  ! something varies
132 end do                  ! mfilms
133
134 mvsav = mv              ! convenience
135 mbien = mmbent(is)      ! quantity
136 write (iplt,212) mbien
137
138 do mbn=1,mbien          ! ambients
139     ias = ias+1
140     mrpeat = mrpeat(ias)
141     imbien = iibent(ias) ! specify ambient
142     imixtr = mixmbn(imbien) ! mixture used as ambient
143     mixflm(mfilms+1) = imixtr
144     mv = mvsav
145
146     if (choice.eq.1) then
147         if (kmix.eq.imixtr) then ! referenced
148             kmix = -kmix        !      negative
149         end if
150     end if
151
152     write (iplt,213) mrpeat, imbien
153
154     mvlmn = mvlmnt(imixtr)      ! vary
155     if (mvlmn.ne.0) then        !      fractions
156         first = .true.

```

```

157      mmlmn = mmlmnt(imixtr)
158      kk      = kklmnt(imixtr)      !      offset
159      do lmn=1,mmlmn                !      fractions
160          kk = kk+1
161          if (lflmnt(kk).eq.1) then !      vary
162              j = mfilmz+kk
163              if (first) then      !      constraint, dv(1)
164                  first = .false.
165              else if (iptw(j).eq.0) then
166                  mv = mv+1      !      local, compress
167                  iptw(j) = mv
168                  iptx(mv) = j
169              end if
170          end if      ! vary
171      end do      ! fractions
172  end if      ! something varies
173
174  mvpar = mvparm(imixtr)      ! vary
175  if (mvpar.ne.0) then      !      parameters
176      mrpar = mrparm(imixtr)
177      kr      = krparm(imixtr)      !      offset
178      do irp=1,mrpar
179          kr = kr+1
180          ip = jrparm(kr)      !      specify index
181          if (lrparm(ip).eq.1) then
182              j = mfilmz+mlmnts+ip
183              if (iptw(j).eq.0) then !      unique
184                  mv = mv+1
185                  iptw(j) = mv
186                  iptx(mv) = j
187              end if
188          end if
189      end do
190  end if
191
192  mm = mmixtr+imbien      ! offset, ambient
193  mvpar = mvparm(mm)      ! vary
194  if (mvpar.ne.0) then      !      parameter
195      mrpar = mrparm(mm)      !      quantity
196      kr      = krparm(mm)      !      offset
197      do irp=1,mrpar
198          kr = kr+1      !      offset
199          ip = jrparm(kr)      !      specify index
200          if (lrparm(ip).eq.1) then !      vary
201              j = mfilmz+mlmnts+ip !      global
202              if (iptw(j).eq.0) then !      unique
203                  mv = mv+1      !      local, compress, aa
204                  iptw(j) = mv
205                  iptx(mv) = j
206              end if
207          end if
208      end do
209  end if      ! something varies

```

```

210
211      mvvari = mv                      ! local quantity
212      firstv = .true.                  ! yet need row: delta
213
214      if (mv.gt.1) then                 ! vary only (0,1) things
215          write (iout,214) mv, mbn, is
216          stop
217      end if
218      if (mrpeat.ne.1) then              ! convenience
219          write (iout,215) mrpeat, mbn, is
220      end if
221
222  c*      do irpeat=1,mrpeat              ! repeats
223  c*          iras = iras+1
224  c*          mexpt = mmexpt(iras)
225          mexpt = mang*mexpt            ! measurements
226          ixpts = 0                     ! reset
227
228          mu = 2                         ! columns of output
229          if (choice.eq.1) then           ! dielectric fcn
230              write (iplt,223) mevs, mang, mu, mexpt
231          else if (choice.eq.2) then      ! x.dat
232              write (iplt,222) mexpt
233          else                            ! values, Jacobians
234              write (iplt,223) mevs, mang, mu, mexpt
235          end if
236
237  c*      do ixpt=1,mexpt                 ! measurements
238  c*          ixpts = ixpts+1
239  c*          wavln1 = wavlns(ixpts)      ! -nm, +eV
240  c*          wavln2 = wavlnu(ixpts)
241  c*          angle1 = angles(ixpts)      ! radians
242  c*          angle2 = anglen(ixpts)
243  c*          psi1 = psiiiis(ixpts)      ! radians
244  c*          psi2 = psiiiu(ixpts)
245  c*          delta1 = deltas(ixpts)      ! radians
246  c*          delta2 = deltau(ixpts)
247
248  c      -----! grid scan
249      do iang=1,mang                     ! incident angles
250          if (iang.eq.mang .and. mang.ne.1) then
251              angl = ang2
252          else
253              angl = angl + ang3*float (iang-1) ! degrees
254          end if
255          angle1 = angl*pi/180.0          ! radians
256          angle2 = 0.01                  ! degrees
257          do ievs=1,mevs                 ! photon energy
258              if (ievs.eq.mevs .and. mevs.ne.1) then
259                  energy = ev2
260              else
261                  energy = ev1 + ev3*float (ievs-1)! eV
262              end if

```

```

263      wavln1 = -wavlev/energy      !      -nm, +eV
264      wavln2 = 0.1                !      convenience
265  c      -----
266      ixpts = ixpts+1              !      update
267
268      do m=1,mfilma                ! initialize, indicate
269          i = mixflm(m)
270          firstx(i) = .true.       !      need of evaluation
271      end do
272
273  c      Discern:      dielectric functions (z)
274
275      imixtr = mixmbn(imbien)       ! ambient
276      firstx(imixtr) = .false.
277      call diefcn (imbien, imixtr, angle1, wavln1,
278          &      dielec( imixtr), dielew( imixtr),
279          &      dielff(1,imixtr),
280          &      dielpp(1,imixtr), dielpa(1,imixtr))
281
282      izes = izes-mzs               ! reset pointer
283      do m=1,mfilms
284          if (m.ne.mfilms) then     ! skip widths
285              izes = izes+1
286          end if
287          izes = izes+1
288          imixtr = iifilm(izes)
289          if (firstx(imixtr)) then   ! first
290              firstx(imixtr) = .false.
291              call diefcn (imbien, imixtr,
292                  &      angle1, wavln1,
293                  &      dielec( imixtr), dielew( imixtr),
294                  &      dielff(1,imixtr),
295                  &      dielpp(1,imixtr), dielpa(1,imixtr))
296          end if
297          die(m) = dielec(imixtr)
298      end do                        ! films
299
300      isampl = is
301      izsmpl = izes-mzs             ! reset index
302      call scatrr (wavln1, angle1,
303          &      isampl, izsmpl, imbien, mvari)
304
305  c      -----
306      if (choice.eq.1) then         ! dielectric
307          if (kmix.lt.0) then       !      referenced
308              delta = real (dielec (-kmix))
309              psi = aimag (dielec (-kmix))
310              write (iplt,311)
311          &      ixpts, energy, angl, delta, psi
312          else if (ixpts.eq.1) then !      notify
313              write (iout,144) is, mbn, kmix
314          end if
315  c      -----

```

```

316      else if (choice .eq.2) then          ! (Delta, psi)
317          psi = b(1)*raddeg                ! degrees
318          delta = b(2)*raddeg
319
320          if (delta.lt.0.0) then            ! [0, 360)
321              delta = delta + 360.0
322          end if
323          if (delta.gt.360.0) then          ! [0, 360)
324              delta = delta - 360.0
325          end if
326          if (delta.ne.0.0) then            ! Nebraska
327              delta = 360.0 - delta        ! convention
328          end if
329
330      write (iplt,321)
331          ixpts, energy, angl, delta, psi
332  c*  &          ixpts, wavln1, angl, delta, psi
333  c          ! convenience
334          du = 0.01                        ! degrees
335          pu = 0.01                        ! degrees
336          write (iplt,322) wavln2, angle2, du, pu
337  c  -----
338      else if (choice .eq.3) then          ! (Delta, psi)
339          psi = b(1)*raddeg                ! degrees
340          delta = b(2)*raddeg
341
342          if (delta.lt.0.0) then            ! [0, 360)
343              delta = delta + 360.0
344          end if
345          if (delta.gt.360.0) then          ! [0, 360)
346              delta = delta - 360.0
347          end if
348          if (delta.ne.0.0) then            ! Nebraska
349              delta = 360.0 - delta        ! convention
350          end if
351
352      write (iplt,331)
353          ixpts, energy, angl, delta, psi
354  c  -----
355      else if (choice.eq.4) then            ! d/d(z,f,p)
356          if (mv.eq.1) then
357              psi = a(1)*raddeg            ! degrees
358              delta = a(2)*raddeg
359          else
360              stop
361          end if
362
363      write (iplt,341)
364          ixpts, energy, angl, delta, psi
365  c  -----
366      else if (choice.eq.5) then            ! d/da
367          psi = c(1)*raddeg                ! degrees
368          delta = c(2)*raddeg

```



```

369
370         write (iplt,361)
371     &         ixpts, energy, angl, delta, psi
372 c         -----
373         else if (choice.eq.6) then                ! d/dE
374             psi  = c(3)*raddeg                    ! degrees
375             delta = c(4)*raddeg
376
377         write (iplt,361)
378     &         ixpts, energy, angl, delta, psi
379 c         -----
380         end if
381
382         end do      ! energy
383     end do          ! angles of incidence
384 c*                end do      ! measurements
385 c*                end do      ! repeats
386
387         if (mv.gt.mvsav) then    ! reset unique-ness
388             mv1 = mvsav+1
389             do i=mv1,mv
390                 j = iptx(i)      ! point to:   iptw
391                 iptw(j) = 0      ! unique-ness
392                 iptx(i) = 0
393             end do
394         end if
395     end do          ! ambients
396
397         if (mvsav.ne.0) then      ! reset unique-ness
398             do i=1,mvsav
399                 j = iptx(i)      ! point to:   iptw
400                 iptw(j) = 0      ! unique-ness
401                 iptx(i) = 0
402             end do
403         end if
404     end do          ! sample
405
406     return
407
408     141 format (/ ' Enter:   kmix " effective medium of',
409     &         ' dielectric function')
410     142 format ( '           kmix "', i3 /)
411     143 format (/ ' ... oops, inconsistent')
412     144 format (/ ' scato2, ... oops,          sample "', i3
413     &         ' ambient "', i3
414     &         ' does not contain mixture "', i3)
415
416     211 format (1x, i5, 15x, 'msamp1')
417     212 format (1x, i5, 15x, 'mbien ')
418     213 format (1x, 2i5, 10x, 'mrpeat, imbien')
419     214 format ( ' ... oops, vary only zero or one thing at a time'
420     &         ' you are assuming:      mvari "', i4
421     &         ' for the case of:      ambient "', i4

```

```

422      &      /'                                sample ', i4)
423  215 format (' ... oops, only one repeat of experiment is necessary'
424      &      /'                                you are assuming:  mrpeat ', i4
425      &      /'                                for the case of:   ambient ', i4
426      &      /'                                sample ', i4 /)
427
428  221 format (1x, 2i5, 10x, 'nx,nu /(i,x,u)')
429  222 format (1x,  i5, 10x, 'mexpt " measurements')
430  223 format (1x, 4i5, 10x, 'nx,ny,nu, (nx*ny) /(i,x,y,u)')
431
432  311 format (1x, i5, 2x, 1p4e13.5, 2x, '(i,E,a, er,ei)')
433  321 format (1x, i5, 2x, 1p4e13.5, 2x, '(i,E,a,  d,p)')
434  322 format (      8x, 1p4e13.5, 2x, '(uncertainty)')
435  331 format (1x, i5, 2x, 1p4e13.5, 2x, '(i,E,a,  d,p)')
436  341 format (1x, i5, 2x, 1p4e13.5, 2x, '(i,E,a, d/db (d,p)')
437  351 format (1x, i5, 2x, 1p4e13.5, 2x, '(i,E,a, d/da (d,p)')
438  361 format (1x, i5, 2x, 1p4e13.5, 2x, '(i,E,a, d/dE (d,p)')
439
440      end

```

6.2.8 SCAN01.FOR

```

1      subroutine scan01                      ! adapted from:  SCAN02
2  c                                         !      called by:  SCATOS
3  c      -----
4  c      Scan the domain grid of model parameters (z,f,p)
5  c      to the set of ellipsometric equations governing experiment.
6  c      Here, we set up the structure of do-loops necessary for the scan.
7  c      Inside the do-nest, we solve the direct or forward problem.
8  c      -----
9
10     include  'iounit.'
11     include  'defnit.'
12     include  'filmmm.'
13     include  'arrays.'
14     include  'nest01.'                      ! do-nest, SEEK02
15     include  'handyy.'                      ! pi
16
17     logical  lbdry, local, first
18     character bufft*8, buffd*9, buffc(9)*1, buff*1, blank*1
19     equivalence (buffd,buffc(1))
20
21     data      blank /' '/
22
23
24     if (mvary.eq.0 .or. mvary.gt.2) then      ! some model parameter
25         write (iout,101)                      !      ought to vary
26         stop
27     end if
28
29  c      Input grid specifications for model parameters (z,p,f).
30
31     write (iout,102)
32     i = 0                                     ! index of vary parameters
33     k = 0                                     ! index for convenience
34  c      -----
35     if (mfilmz .ne. 0) then                      ! widths
36         local = .true.                          ! first
37         do m=1,mfilmz
38             if (lwidth(m).eq.1 .and. iptw(m).ne.-1) then ! vary + utilized
39                 if (local) then                  ! first
40                     local = .false.
41                     write (iout,111)              ! Enter: widths
42                 end if
43                 i = i+1                          ! vary
44                 k = k+1                          ! convenience
45
46                 read  ( inn, *)      j, z1, z2, z3
47                 write (iout,112) k, j, z1, z2, z3, i
48
49                 if ( j.ne.m .or. z2.le.z1 .or.
50 *                 z1.lt.0.0 .or. z2.lt.0.0 .or. z3.lt.0.0) then

```

```

51         write (iout,113)
52         stop
53     end if
54
55     ppp1(i) = z1
56     ppp2(i) = z2
57
58     if (z3 .eq. 0.0) then
59         iii2(i) = 2
60         ppp3(i) = z2-z1
61     else
62         iii2(i) = 1 + nint ((z2-z1)/z3)
63         ppp3(i) = (z2-z1) /float (max (1, iii2(i)-1))
64     end if
65
66     psav(i) = widths(m)
67     end if      ! utilized + vary
68     end do      ! mfilmz
69 end if
70 c -----
71 c Since ordering in PPP assumes (z,f,p) rather than (z,p,f),
72 c and if we impose the same ordering of groups as in X.DAT,
73 c then we must account for this interchange of group ordering.
74 c Method: pre-index the 'vary' volume fractions.
75
76 ipsav1 = i                ! retain last value of index
77 do m=1,mmixtr             ! effective media
78     mmlmn = mmlmnt(m)
79     mvlmn = mvlmnt(m)
80     kk = kklmnt(m)
81     if (mvlmn .ne. 0) then                ! vary
82         j = mfilmz+kk+1
83         if (iptw(j).ne.-1) then            ! utilized
84             first = .true.
85             do lmn=1,mmlmn
86                 kk = kk+1
87                 if (lflmnt(kk).eq.1) then    ! vary
88                     if (first) then          ! skip
89                         first = .false.
90                     else
91                         i = i+1                ! hop
92                     end if      ! first
93                 end if      ! vary
94             end do      ! fractions
95         end if      ! utilized
96     end if      ! something varies
97 end do      ! mixtures
98 c -----
99 if (mrpars .ne. 0) then                ! parameters
100     local = .true.                    ! first
101     do m=1,mrpars
102         j = mfilmz+mlmnts+m
103         if (lrparm(m).eq.1 .and. iptw(j).ne.-1) then

```

```

104         if (local) then
105             local = .false.
106             write (iout,131)
107         end if
108         i = i+1                                ! vary
109         k = k+1                                ! convenience
110
111         read ( inn, *)      j, p1, p2, p3
112         write (iout,132) k, j, p1, p2, p3, i
113
114         if (j.ne.m .or. p2.le.p1 .or. p3.lt.0.0) then
115             write (iout,133)
116             stop
117         end if
118
119         ppp1(i) = p1
120         ppp2(i) = p2
121
122         if (p3 .eq. 0.0) then
123             iii2(i) = 2
124             ppp3(i) = p2-p1
125         else
126             iii2(i) = 1 + nint ((p2-p1)/p3)
127             ppp3(i) = (p2-p1) /float (max (1, iii2(i)-1))
128         end if
129
130         psav(i) = rrparm(m)
131     end if
132 end do
133 end if
134 ipsav2 = i                                ! retain last value of index
135 c -----
136 i = ipsav1                                ! recover initial indexing
137 local = .true.                            ! first
138 do m=1,mmixtr                            ! fractions
139     mmlmn = mmlmnt(m)
140     mvlmn = mvlmnt(m)
141     kk = kklmnt(m)
142     if (mvlmn .ne. 0) then                ! vary
143         j = mfilmz+kk+1
144         if (iptw(j).ne.-1) then            ! utilized
145             if (local) then                ! first
146                 local = .false.
147                 write (iout,121)
148             end if
149             first = .true.
150             do lmn=1,mmlmn
151                 kk = kk+1
152                 if (lflmnt(kk).eq.1) then    ! vary
153                     if (first) then          ! skip
154                         first = .false.
155                     else
156                         i = i+1                ! vary

```



```

157         k = k+1                                ! convenience
158
159         read ( inn, *)      j, f1, f2, f3
160         write (iout,122) k, j, f1, f2, f3, i
161
162         if ( j.ne.lmn .or. f2.le.f1 .or.
163             &      f1.lt.0.0 .or. f2.lt.0.0 .or.
164             &      f3.lt.0.0 .or. f2.gt.1.0      ) then
165             write (iout,123)
166             stop
167         end if
168
169         ppp1(i) = f1
170         ppp2(i) = f2
171
172         if (f3 .eq. 0.0) then
173             iii2(i) = 2
174             ppp3(i) = f2-f1
175         else
176             iii2(i) = 1 + nint ((f2-f1)/f3)
177             ppp3(i) = (f2-f1) /
178             &      float (max (1, iii2(i)-1))
179         end if
180
181         psav(i) = fflmnt(kk)
182         end if      ! first
183         end if      ! vary
184         end do      ! fractions
185         end if      ! utilized
186         end if      ! something varies
187         end do      ! mixtures
188     c -----
189     i = ipsav2      ! recover last value of indexing
190     if (mvary .ne. i) then      ! depth of do-loop nest, ARRANG
191         write (iout,135)
192         stop
193     end if
194
195     c -----
196     c* write (iout,141)      ! optimization strategies
197     c* read ( inn, *)  ichoic      ! 0,1
198     c* write (iout,142)  ichoic
199     c* if (ichoic.lt.0 .or. ichoic.gt.1) then
200     c*     write (iout,143)
201     c*     stop
202     c* end if      ! NO optimization
203
204     c -----
205     c Discern breakpoints ... from previous attempts
206
207     write (iout,151)
208     read ( inn,*,err=11,end=11) mvarii, kts, ktm, old
209     write (iout,152)      mvarii, kts, ktm, old

```

```

210
211      if (mvarii.ne.mvary .or. old.ls.0.0 .or.
212      &    kts.lt.1          .or. ktm.lt.1      ) goto 11
213
214      write (iout,153)
215      do i=1,mvary
216          read ( inn,*,err=11,end=11)  j, iiii(i), pppp(i), psav(i)
217          write (iout,154)              j, iiii(i), pppp(i), psav(i)
218
219          if (iiii(i) .lt. 1          .or. j.ne.i .or.
220      &      iiii(i) .gt. iii2(i)          .or.
221      &      pppp(i) .lt. ppp1(i)-ppp3(i)*0.001 .or.
222      &      pppp(i) .gt. ppp2(i)+ppp3(i)*0.001 .or.
223      &      psav(i) .lt. ppp1(i)-ppp3(i)*0.001 .or.
224      &      psav(i) .gt. ppp2(i)+ppp3(i)*0.001      ) then
225              write (iout,155)
226              stop
227          end if
228
229          if (iiii(i).lt.iii2(i) .or. iii2(i).eq.1) then
230              ppppi = ppp1(i) + ppp3(i)*float(iiii(i)-1)      ! []
231          else
232              ppppi = ppp2(i)                                  ! ]
233          end if
234
235          if (abs(pppp(i)-ppppi) .gt. ppp3(i)*0.01) then
236              write (iout,156)
237              stop
238          end if
239      end do
240
241      write (iout,161)
242      iiistp = 1                      ! do-increment
243      iii = mvary                      ! depth of do-nest
244      it1 = iftime(i)                 ! start clock
245      goto 2
246 11 continue
247      write (iout,162)
248      it1 = iftime(i)                 ! start clock
249
250  c -----
251  c Formulate header card for the plot utility.
252  c Plot format:      nx,ny,nu /(i,x,y,u)  ==> index backwards
253
254      m = 1
255      kt = mvary+1
256      if (mvary .eq. 1) then
257          write (iplt,212) (iii2(kt-j), j=1,mvary), m      ! header card
258      else
259          write (iplt,213) (iii2(kt-j), j=1,mvary), m      ! header card
260      end if
261
262  c -----

```

```

263 c      Emulate, initialize, activate:   the nest of do-loops
264
265      do i=1,mvary
266          iiii(i) = 0                      ! i1-i3
267      end do
268
269      kts = 0                              ! counter
270      iiistp = 1                          ! do-increment
271      iii = 0                             ! index do-levels
272      1 iii = iii+1                        ! index of:   iii-th level
273      if (iii .gt. mvary) goto 3
274      2 iiii(iii) = iiii(iii) + iiistp      ! update do parameter
275      if (iiiii(iii) .lt. iii2(iii)) then   ! test upper limit
276          pppp(iii) = ppp1(iii) + ppp3(iii)*float (iiiii(iii) -1)
277          goto 1
278      else if (iiiii(iii) .eq. iii2(iii)) then
279          if (iii2(iii) .eq. 1) then
280              pppp(iii) = ppp1(iii)
281          else
282              pppp(iii) = ppp2(iii)
283          end if
284          goto 1
285      end if
286      iiii(iii) = 0                        ! i1-i3, reset inner do
287      iii = iii-1                          ! backup one do-level
288      if (iii.eq.0) goto 4                 ! escape do-nest
289      goto 2
290      3 iii = iii-1                        ! level of inner-most do.
291 c      -----
292      kts = kts+1                          ! simple counter
293
294 c      Reset the model parameters to their appropriate values.
295
296      do i=1,mvary
297          j = iptu(i)
298          if (j .le. mfilmz) then
299              widths(j) = pppp(i)
300          else if (j .le. mfilmz+mlmnts) then
301              j = j-mfilmz
302              fflmnt(j) = pppp(i)
303          else
304              j = j-mfilmz-mlmnts
305              rrparm(j) = pppp(i)
306          end if
307      end do
308
309      do m=1,mmixtr                          ! mixtures
310          mvlmn = mvlmnt(m)
311          if (mvlmn.ne.0) then                ! vary
312              mmlmn = mmlmnt(m)
313              kk = kklmnt(m)                  ! offset
314              j = mfilmz+kk+1
315              if (iptw(j).ne.-1) then          ! utilized

```

```

316          fu = 0.0
317          fv = 0.0
318          first = .true.
319          do lmn=1,mmlmn                                ! fractions
320              kk = kk+1
321              if (lflmnt(kk).eq.1) then                    ! vary
322                  if (first) then
323                      first = .false.
324                      kk1 = kk
325                  else
326                      fv = fv+fllmnt(kk)
327                  end if
328              else                                          ! froz
329                  fu = fu+fllmnt(kk)
330              end if
331          end do      ! fractions
332          fllmnt(kk1) = 1.0-fu-fv                            ! constraint
333      end if      ! utilized
334  end if      ! vary
335  end do      ! mixture
336  c  -----
337  c*  if (ichoic.eq.1) then
338  c*      call seeko2                                ! constrained optimization
339  c*  end if
340
341  llnorm = .false.
342  call asmb10                                ! residual only, |g|.
343  call norm (meqns, bb, bnorm, 1) ! retain norm of residual
344  bnorm = bnorm *180.0/pi                ! degrees <--- radians
345
346  c  -----
347  m = mvary+1                                ! backwards
348  write (iplt,214) kts, (pppp(m-j), j=1,mvary), bnorm
349
350  c  -----
351  if (kts .eq. 1) then                        ! first
352      ktm = 1                                ! density of states along minimum
353      old = bnorm
354      do i=1,mvary
355          j = iptu(i)
356          if (j .le. mfilmz) then
357              psav(i) = widths(j)
358          else if (j .le. mfilmz+mlmnts) then
359              j = j-mfilmz
360              psav(i) = fllmnt(j)
361          else
362              j = j-mfilmz-mlmnts
363              psav(i) = rrparm(j)
364          end if
365      end do
366  else if (bnorm .lt. old) then
367      ktm = 1                                ! density of states along minimum
368      old = bnorm

```

```

369         do i=1,mvary
370             j = iptu(i)
371             if (j .le. mfilmz) then
372                 psav(i) = widths(j)
373             else if (j .le. mfilmz+mlmnts) then
374                 j = j-mfilmz
375                 psav(i) = fflmnt(j)
376             else
377                 j = j-mfilmz-mlmnts
378                 psav(i) = rrparm(j)
379             end if
380         end do
381     else if (bnorm .eq. old) then
382         ktm = ktm+1                                ! density of states along minimum
383     end if
384
385     it2 = iftime (i)                                ! CPU clock
386     tim = float (it2-it1) /6.0E4                    ! CPU minutes elapsed
387
388     if (tim .gt. 15.0) then                            ! breakpoint
389         it1 = it2
390         open (unit=isout, file='x.sout', status='unknown')
391         write (isout,171) mvary, kts, ktm, old
392         do i=1,mvary
393             write (isout,172) i, iiii(i), pppp(i), psav(i)
394         end do
395         call time (bufft)                            ! hh:mm:ss
396         call date (buffd)                            ! dd-mmm-yy
397
398         buff = buffc(1)                              ! interchange (dd,yy)
399         buffc(1) = buffc(8)
400         buffc(8) = buff
401         buff = buffc(2)
402         buffc(2) = buffc(9)
403         buffc(9) = buff
404
405         write (isout,173) bufft, buffd                ! convenience
406         close (unit=isout)
407     end if
408 c -----! finish processing body
409     goto 2                                            ! nested do-loop: iiii
410 4 continue                                          ! last line of do-nest, iiii
411 c =====
412
413     lbdry = .false.
414
415     write (iout,181) kts, ktm, old                    ! DOS along minimum
416     write (iout,182)
417
418     do i=1,mvary
419         local = (psav(i) .le. ppp1(i)+ppp3(i)*0.001) .or.
420 &             (psav(i) .ge. ppp2(i)-ppp3(i)*0.001)
421 c*         local = local .and. (iii2(i).ne.1)

```



```

422      lbdry = lbdry .or. local                ! retain hitting boundary
423      j = iptu(i)
424
425      if (j .le. mfilmz) then
426          widths(j) = psav(i)
427          if (local) then
428              write (iout,183) i, psav(i), j, blank
429          else
430              write (iout,183) i, psav(i), j
431          end if
432      else if (j .le. mfilmz+mlmnts) then
433          j = j-mfilmz
434          fflmnt(j) = psav(i)
435          if (local) then
436              write (iout,184) i, psav(i), j, blank
437          else
438              write (iout,184) i, psav(i), j
439          end if
440      else
441          j = j-mfilmz-mlmnts
442          rrparm(j) = psav(i)
443          if (local) then
444              write (iout,185) i, psav(i), j, blank
445          else
446              write (iout,185) i, psav(i), j
447          end if
448      end if
449  end do                                ! vary
450
451  do m=1,mmixtr                          ! mixtures
452      mvlmn = mvlmnt(m)
453      if (mvlmn.ne.0) then                ! vary
454          mmlmn = mmlmnt(m)
455          kk      = kklmnt(m)
456          j = mfilmz+kk+1
457          if (iptw(j).ne.-1) then          ! utilized
458              fu = 0.0
459              fv = 0.0
460              first = .true.
461              do lmn=1,mmlmn                ! fractions
462                  kk = kk+1
463                  if (lflmnt(kk).eq.1) then ! vary
464                      if (first) then
465                          first = .false.
466                          kk1 = kk
467                      else
468                          fv = fv+fflmnt(kk)
469                      end if
470                  else                        ! froz
471                      fu = fu+fflmnt(kk)
472                  end if
473              end do                        ! fractions
474              fflmnt(kk1) = 1.0-fu-fv      ! constraint

```

```

475         end if          ! utilized
476     end if          ! vary
477 end do          ! mixture
478
479 if (lbdry) write (iout,186)
480 c -----
481
482 call corlat
483 call scato1 (3)
484
485 return
486
487 101 format (/ ' oops, all model parameters are frozen, or '
488 & / ' too many model parameters are varying.'
489 & / ' For convenience, only 1 or 2 may vary.')
490 102 format (/ ' Scan a grid of model parameters: (z,p,f). '
491 & / ' Grid info: DO-loop parameters '
492 & / ' Grid info:', 4x, 'i,', 8x,
493 & 'initial,', 6x, 'final,', 5x, 'increment' )
494
495 111 format (/ ' Enter: i, z1, z2, z3 (widths) ')
496 112 format (3x,i4, ' '), 3x, i5, 3x, 3f13.4, 5x, '(', i3, ')')
497 113 format (/ ' oops, inconsistent data input ')
498
499 121 format (/ ' Enter: i, f1, f2, f3 (fraction) ')
500 122 format (3x,i4, ' '), 3x, i5, 3x, 3f13.4, 5x, '(', i3, ')')
501 123 format (/ ' oops, inconsistent data input ')
502
503 131 format (/ ' Enter: i, p1, p2, p3 (parameters) ')
504 132 format (3x,i4, ' '), 3x, i5, 3x, 1p3e13.4, 5x, '(', i3, ')')
505 133 format (/ ' oops, inconsistent data input ')
506
507 135 format (/ ' oops, inconsistent info: mvary')
508
509 141 format (/ ' Enter: option regarding the grid scan:'
510 & / ' 0, no optimization, |g| only,'
511 & / ' 1, full optimization, Jacobian.')
512 142 format ( ' option ', i1)
513 143 format (/ ' oops, inconsistent data input ')
514
515 151 format (/ ' Restart by attempting to read breakpoint info')
516 152 format ( 1x, 3i10, 1p15.6, 5x, '(mvary, kts, ktm, residual)')
517 153 format (/ ' Enter: i, ip, pp, psav (breakpoint info) ')
518 154 format ( 1x, 2(i4,1x), 1p2e15.6 )
519 155 format (/ ' oops, your attempt at restarting has failed.')
520 156 format (/ ' oops, your attempt at restarting has failed.')
521
522 161 format ( ' Good, your attempt at restarting was successful.')
523 162 format (/ ' Note: NO attempt was made to restart.')
524
525 171 format (1x, i4,1x, 2i10, 1p1e15.6, 5x, ' mvary,kts,ktm,residual')
526 172 format (1x, 2(i4,1x), 1p2e15.6, 5x, ' i, ip, p, p(min) ')
527 173 format ( ' wall clock: time = ', a8, ' ' hh:mm:ss'

```

```

528      &      /'      date = ', a9, ' ^ yy-mmm-dd' )
529
530      181 format (/ ' number of grid points scanned, kts =', i10
531      &      /'      population along the minimum, ktm =', i10
532      &      /'      norm of the residual, |g| =', 1pe13.5,
533      &      ' (degrees)' )
534      182 format (/ ' model parameter value along the minimum:')
535      183 format (1x, i4, ')', 1pe15.5, ', for:', i5, ', (z)',
536      &      a1, ' ^ boundary')
537      184 format (1x, i4, ')', 1pe15.5, ', for:', i5, ', (f)',
538      &      a1, ' ^ boundary')
539      185 format (1x, i4, ')', 1pe15.5, ', for:', i5, ', (p)',
540      &      a1, ' ^ boundary')
541      186 format (/ ' Note:      minimum point is near a boundary.')
542
543      212 format ( 1x, 2i5, ' ^ mx, mu /(i, x, |g|) ')
544      213 format ( 1x, 3i5, ' ^ mx(2), mx(1), mu /(i, x(2), x(1), |g|)')
545      214 format ( 1x, i6, 1p3e15.6)
546      end

```

6.2.9 SCANO2.FOR

```

1      subroutine scano2
2
3      c -----
4      c Scan the domain grid of model parameters (z,f,p)
5      c to the set of ellipsometric equations governing experiment.
6      c Minimize the sum of error residuals in the least-squares sense.
7      c Method of solution: damped least-squares analysis.
8      c Here, we set up the structure of do-loops necessary for the scan.
9      c Inside the do-nest, we solve the direct or forward problem.
10     c -----
11
12     include 'iounit.'
13     include 'defnit.'
14     include 'filmm.'
15     include 'arrays.'
16     include 'nesto1.'          ! do-nest, SEEK02
17     include 'handyy.'          ! pi
18
19     logical lbdry, local, first
20     character bufft*8, buffd*9, buffc(9)*1, buff*1, blank*1
21     equivalence (buffd,buffc(1))
22
23     data blank /' '/
24
25
26     if (mvary .eq. 0) then          ! something needs to vary
27         write (iout,101)
28         stop
29     end if
30
31     c Input grid specifications for model parameters (z,p,f).
32
33     write (iout,102)
34     i = 0          ! index of vary parameters
35     k = 0          ! index for convenience
36     c -----
37     if (mfilmz .ne. 0) then          ! widths
38         local = .true.              ! first
39         do m=1,mfilmz
40             if (lwidth(m).eq.1 .and. iptw(m).ne.-1) then ! vary + utilized
41                 if (local) then          ! first
42                     local = .false.
43                     write (iout,111)      ! Enter: widths
44                 end if
45                 i = i+1                  ! vary
46                 k = k+1                  ! convenience
47
48                 read ( inn, *)          j, z1, z2, z3
49                 write (iout,112) k, j, z1, z2, z3, i
50

```

```

51         if ( j.ne.m .or. z2.le.z1 .or.
52 &          z1.lt.0.0 .or. z2.lt.0.0 .or. z3.lt.0.0) then
53             write (iout,113)
54             stop
55         end if
56
57         ppp1(i) = z1
58         ppp2(i) = z2
59
60         if (z3 .eq. 0.0) then
61             iii2(i) = 2
62             ppp3(i) = z2-z1
63         else
64             iii2(i) = 1 + nint ((z2-z1)/z3)
65             ppp3(i) = (z2-z1) /float (max (1, iii2(i)-1))
66         end if
67
68         psav(i) = widths(m)
69     end if ! utilized + vary
70 end do ! mfilmz
71 end if
72 c -----
73 c Since ordering in PPP assumes (z,f,p) rather than (z,p,f),
74 c and if we impose the same ordering of groups as in X.DAT,
75 c then we must account for this interchange of group ordering.
76 c Method: pre-index the 'vary' volume fractions.
77
78 ipsav1 = i ! retain last value of index
79 do m=1,mmixtr ! effective media
80     mmlmn = mmlmnt(m)
81     mvlmn = mvlmnt(m)
82     kk = kklmnt(m)
83     if (mvlmn .ne. 0) then ! vary
84         j = mfilmz+kk+1
85         if (iptw(j).ne.-1) then ! utilized
86             first = .true.
87             do lmn=1,mmlmn
88                 kk = kk+1
89                 if (lflmnt(kk).eq.1) then ! vary
90                     if (first) then ! skip
91                         first = .false.
92                     else
93                         i = i+1 ! hop
94                     end if ! first
95                 end if ! vary
96             end do ! fractions
97         end if ! utilized
98     end if ! something varies
99 end do ! mixtures
100 c -----
101 if (mrpars .ne. 0) then ! parameters
102     local = .true. ! first
103     do m=1,mrpars

```



```

104      j = mfilmz+mlmnts+m
105      if (lrparm(m).eq.1 .and. iptw(j).ne.-1) then
106          if (local) then
107              local = .false.
108              write (iout,131)
109          end if
110          i = i+1                                ! vary
111          k = k+1                                ! convenience
112
113          read ( inn, *)      j, p1, p2, p3
114          write (iout,132) k, j, p1, p2, p3, i
115
116          if (j.ne.m .or. p2.le.p1 .or. p3.lt.0.0) then
117              write (iout,133)
118              stop
119          end if
120
121          ppp1(i) = p1
122          ppp2(i) = p2
123
124          if (p3 .eq. 0.0) then
125              iii2(i) = 2
126              ppp3(i) = p2-p1
127          else
128              iii2(i) = 1 + nint ((p2-p1)/p3)
129              ppp3(i) = (p2-p1) /float (max (1, iii2(i)-1))
130          end if
131
132          psav(i) = rrparm(m)
133      end if
134  end do
135  end if
136  ipsav2 = i                                ! retain last value of index
137  c -----
138  i = ipsav1                                ! recover initial indexing
139  local = .true.                            ! first
140  do m=1,mnixtr                            ! fractions
141      mmlmn = mmlmnt(m)
142      mvlmn = mvlmnt(m)
143      kk = kklmnt(m)
144      if (mvlmn .ne. 0) then                ! vary
145          j = mfilmz+kk+1
146          if (iptw(j).ne.-1) then            ! utilized
147              if (local) then                ! first
148                  local = .false.
149                  write (iout,121)
150              end if
151              first = .true.
152              do lmn=1,mmlmn
153                  kk = kk+1
154                  if (lflmnt(kk).eq.1) then    ! vary
155                      if (first) then          ! skip
156                          first = .false.

```

```

157         else
158             i = i+1                                ! vary
159             k = k+1                                ! convenience
160
161             read ( inn, *)      j, f1, f2, f3
162             write (iout,122) k, j, f1, f2, f3, i
163
164             if ( j.ne.lmn .or. f2.le.f1 .or.
165                 & f1.lt.-0.5 .or. f2.gt.1.5 .or.
166                 & f3.lt. 0.0 ) then
167                 write (iout,123)
168                 stop
169             end if
170
171             ppp1(i) = f1
172             ppp2(i) = f2
173
174             if (f3 .eq. 0.0) then
175                 iii2(i) = 2
176                 ppp3(i) = f2-f1
177             else
178                 iii2(i) = 1 + nint ((f2-f1)/f3)
179                 ppp3(i) = (f2-f1) /
180                 & float (max (1, iii2(i)-1))
181             end if
182
183             psav(i) = fflmnt(kk)
184             end if      ! first
185             end if      ! vary
186             end do      ! fractions
187             end if      ! utilized
188             end if      ! something varies
189             end do      ! mixtures
190 c -----
191 i = ipsav2                ! recover last value of indexing
192 if (mvarry .ne. i) then   ! depth of do-loop nest, ARRANG
193     write (iout,135)
194     stop
195 end if
196
197 c -----
198 write (iout,141)          ! optimization strategies
199 read ( inn, *)  ichoic    ! 0,1
200 write (iout,142)  ichoic
201 if (ichoic.lt.0 .or. ichoic.gt.1) then
202     write (iout,143)
203     stop
204 end if
205
206 c -----
207 c Discern breakpoints ... from previous attempts
208
209 write (iout,151)

```

```

210      read ( inn,*,err=11,end=11) mvarii, kts, ktm, old
211      write (iout,152)              mvarii, kts, ktm, old
212
213      if (mvarii.ne.mvary .or. old.le.0.0 .or.
214      &   kts.lt.1           .or. ktm.lt.1           ) goto 11
215
216      write (iout,153)
217      do i=1,mvary
218          read ( inn,*,err=11,end=11) j, iiii(i), pppp(i), psav(i)
219          write (iout,154)              j, iiii(i), pppp(i), psav(i)
220
221          if (iiii(i) .lt. 1 .or. j.ne.i .or.
222      &       iiii(i) .gt. iiii2(i) .or.
223      &       pppp(i) .lt. ppp1(i)-ppp3(i)*0.001 .or.
224      &       pppp(i) .gt. ppp2(i)+ppp3(i)*0.001 .or.
225      &       psav(i) .lt. ppp1(i)-ppp3(i)*0.001 .or.
226      &       psav(i) .gt. ppp2(i)+ppp3(i)*0.001 ) then
227              write (iout,155)
228              stop
229          end if
230
231          if (iiii(i).lt.iii2(i) .or. iiii2(i).eq.1) then
232              ppppi = ppp1(i) + ppp3(i)*float(iiii(i) -1)      ! [)
233          else
234              ppppi = ppp2(i)                                     ! ]
235          end if
236
237          if (abs(pppp(i)-ppppi) .gt. ppp3(i)*0.01) then
238              write (iout,156)
239              stop
240          end if
241      end do
242
243      write (iout,161)
244      iistp = 1                                                    ! do-increment
245      iii = mvary                                                  ! depth of do-nest
246      it1 = iftime(i)                                              ! start clock
247      goto 2
248 11 continue
249      write (iout,162)
250      it1 = iftime(i)                                              ! start clock
251
252  c -----
253  c Emulate, initialize, activate:  the nest of do-loops
254
255      do i=1,mvary
256          iiii(i) = 0                                              ! i1-i3
257      end do
258
259      kts = 0                                                       ! counter
260      iistp = 1                                                     ! do-increment
261      iii = 0                                                       ! index do-levels
262 1 iii = iii+1                                                     ! index of:  iii-th level

```

```

263     if (iii .gt. mvary) goto 3
264 2  iiii(iii) = iiii(iii) + iiistp           ! update do parameter
265     if (iiii(iii) .lt. iii2(iii)) then      ! test upper limit
266         pppp(iii) = ppp1(iii) + ppp3(iii)*float (iiii(iii) -1)
267         goto 1
268     else if (iiii(iii) .eq. iii2(iii)) then
269         if (iii2(iii) .eq. 1) then
270             pppp(iii) = ppp1(iii)
271         else
272             pppp(iii) = ppp2(iii)
273         end if
274         goto 1
275     end if
276     iiii(iii) = 0                             ! i1-i3, reset inner do
277     iii = iii-1                               ! backup one do-level
278     if (iii.eq.0) goto 4                      ! escape do-nest
279     goto 2
280 3  iii = iii-1                               ! level of inner-most do.
281 c  -----
282     kts = kts+1                             ! simple counter
283
284 c  Reset the model parameters to their appropriate values.
285
286     do i=1,mvary
287         j = iptu(i)
288         if (j .le. mfilmz) then
289             widths(j) = pppp(i)
290         else if (j .le. mfilmz+mlmnts) then
291             j = j-mfilmz
292             fflmnt(j) = pppp(i)
293         else
294             j = j-mfilmz-mlmnts
295             rrparm(j) = pppp(i)
296         end if
297     end do
298
299     do m=1,mmixtr                             ! mixtures
300         mvlmn = mvlmnt(m)
301         if (mvlmn.ne.0) then                   ! vary
302             mmlmn = mmlmnt(m)
303             kk = kklmnt(m)                   ! offset
304             j = mfilmz+kk+1
305             if (iptw(j).ne.-1) then           ! utilized
306                 fu = 0.0
307                 fv = 0.0
308                 first = .true.
309                 do lmn=1,mmlmn               ! fractions
310                     kk = kk+1
311                     if (lflmnt(kk).eq.1) then ! vary
312                         if (first) then
313                             first = .false.
314                             kk1 = kk
315                         else

```

```

316             fv = fv+fflmnt(kk)
317         end if
318     else                                     ! froz
319         fu = fu+fflmnt(kk)
320     end if
321     end do                                     ! fractions
322     fflmnt(kk1) = 1.0-fu-fv                 ! constraint
323 end if                                     ! utilized
324 end if                                     ! vary
325 end do                                     ! mixture
326 c -----
327 if (ichoic.eq.1) then
328     call seeko2                             ! constrained optimization
329 end if
330
331 llnorm = .false.
332 call asmb10                                ! residual only, |g|.
333 call norm (meqns, bb, bnorm, 1)           ! retain norm of residual
334 bnorm = bnorm *180.0/pi                  ! degrees <--- radians
335
336 if (kts .eq. 1) then                       ! first
337     ktm = 1                               ! density of states along minimum
338     old = bnorm
339     do i=1,mvary
340         j = iptu(i)
341         if (j .le. mfilmz) then
342             psav(i) = widths(j)
343         else if (j .le. mfilmz+mlmnts) then
344             j = j-mfilmz
345             psav(i) = fflmnt(j)
346         else
347             j = j-mfilmz-mlmnts
348             psav(i) = rrparm(j)
349         end if
350     end do
351 else if (bnorm .lt. old) then
352     ktm = 1                               ! density of states along minimum
353     old = bnorm
354     do i=1,mvary
355         j = iptu(i)
356         if (j .le. mfilmz) then
357             psav(i) = widths(j)
358         else if (j .le. mfilmz+mlmnts) then
359             j = j-mfilmz
360             psav(i) = fflmnt(j)
361         else
362             j = j-mfilmz-mlmnts
363             psav(i) = rrparm(j)
364         end if
365     end do
366 else if (bnorm .eq. old) then
367     ktm = ktm+1                           ! density of states along minimum
368 end if

```



```

369
370      it2 = iftime (i)                      ! CPU clock
371      tim = float (it2-it1) /6.0E4          ! CPU minutes elapsed
372
373      if (tim .gt. 15.0) then                ! breakpoint
374          it1 = it2
375          open (unit=isout, file='x.sout', status='unknown')
376          write (isout,171) mvary, kts, ktm, old
377          do i=1,mvary
378              write (isout,172) i, iiii(i), pppp(i), psav(i)
379          end do
380          call time (bufft)                  ! hh:mm:ss
381          call date (buffd)                 ! dd-mmm-yy
382
383          buff = buffc(1)                   ! interchange (dd,yy)
384          buffc(1) = buffc(8)
385          buffc(8) = buff
386          buff = buffc(2)
387          buffc(2) = buffc(9)
388          buffc(9) = buff
389
390          write (isout,173) bufft, buffd    ! convenience
391          close (unit=isout)
392      end if
393  c -----! finish processing body
394      goto 2                                ! nested do-loop: iiii
395  4 continue                                ! last line of do-nest, iiii
396  c =====
397
398      lbdry = .false.
399
400      write (iout,181) kts, ktm, old        ! DOS along minimum
401      write (iout,182)
402
403      do i=1,mvary
404          local = (psav(i) .le. ppp1(i)+ppp3(i)*0.001) .or.
405          &      (psav(i) .ge. ppp2(i)-ppp3(i)*0.001)
406  c*      local = local .and. (iii2(i).ne.1)
407          lbdry = lbdry .or. local          ! retain hitting boundary
408          j = iptu(i)
409
410          if (j .le. mfilmz) then
411              widths(j) = psav(i)
412              if (local) then
413                  write (iout,183) i, psav(i), j, blank
414              else
415                  write (iout,183) i, psav(i), j
416              end if
417          else if (j .le. mfilmz+mlmnts) then
418              j = j-mfilmz
419              fflmnt(j) = psav(i)
420              if (local) then
421                  write (iout,184) i, psav(i), j, blank

```

```

422         else
423             write (iout,184) i, psav(i), j
424         end if
425     else
426         j = j-mfilmz-mlmnts
427         rrparm(j) = psav(i)
428         if (local) then
429             write (iout,185) i, psav(i), j, blank
430         else
431             write (iout,185) i, psav(i), j
432         end if
433     end if
434 end do                ! vary
435
436 do m=1,mmixtr                ! mixtures
437     mvlmn = mvlmnt(m)
438     if (mvlmn.ne.0) then                ! vary
439         mmlmn = mmlmnt(m)
440         kk = kklmnt(m)
441         j = mfilmz+kk+1
442         if (iptw(j).ne.-1) then                ! utilized
443             fu = 0.0
444             fv = 0.0
445             first = .true.
446             do lmn=1,mmlmn                ! fractions
447                 kk = kk+1
448                 if (lflmnt(kk).eq.1) then                ! vary
449                     if (first) then
450                         first = .false.
451                         kk1 = kk
452                     else
453                         fv = fv+fvlmnt(kk)
454                     end if
455                 else                ! froz
456                     fu = fu+fvlmnt(kk)
457                 end if
458             end do                ! fractions
459             fvlmnt(kk1) = 1.0-fu-fv                ! constraint
460         end if                ! utilized
461     end if                ! vary
462 end do                ! mixture
463
464 if (lbdry) write (iout,186)
465 c -----
466
467 call corlat
468 call scato1 (3)
469
470 return
471
472 101 format (' oops, all model parameters are frozen, at least'
473 &          /'          one of them must be allowed to vary.      ')
474 102 format (' Scan a grid of model parameters: (z,p,f). ')

```

```

475      &          /' Grid info:  DO-loop parameters
476      &          /' Grid info:', 4x, 'i,',      8x,
477      &          'initial,', 6x, 'final,', 5x, 'increment' )
478
479      111 format (/ Enter:   i, z1, z2, z3           (widths) ')
480      112 format (3x,i4, ')', 3x, i5, 3x, 3f13.4, 5x, '(', i3, ')')
481      113 format (/ oops, inconsistent data input ')
482
483      121 format (/ Enter:   i, f1, f2, f3           (fraction) ')
484      122 format (3x,i4, ')', 3x, i5, 3x, 3f13.4, 5x, '(', i3, ')')
485      123 format (/ oops, inconsistent data input ')
486
487      131 format (/ Enter:   i, p1, p2, p3           (parameters) ')
488      132 format (3x,i4, ')', 3x, i5, 3x, 1p3e13.4, 5x, '(', i3, ')')
489      133 format (/ oops, inconsistent data input ')
490
491      135 format (/ oops, inconsistent info:  mvary')
492
493      141 format (/ Enter:  option regarding the grid scan:'
494      &          /'          0,    no optimization, |g| only,'
495      &          /'          1,    full optimization, Jacobian.')
496      142 format ( ' option      ', i1)
497      143 format (/ oops, inconsistent data input ')
498
499      151 format (/ Restart by attempting to read breakpoint info')
500      152 format ( 1x, 3i10, 1p15.6, 5x, '(mvary, kts, ktm, residual)')
501      153 format (/ Enter:   i, ip, pp, psav          (breakpoint info) ')
502      154 format ( 1x, 2(i4,1x), 1p2e15.6 )
503      155 format (/ oops, your attempt at restarting has failed.')
504      156 format (/ oops, your attempt at restarting has failed.')
505
506      161 format ( ' Good, your attempt at restarting was successful.')
507      162 format (/ Note:    NO attempt was made to restart.'/)
508
509      171 format (1x, i4,1x, 2i10, 1p1e15.6, 5x, ' mvary,kts,ktm,residual')
510      172 format (1x, 2(i4,1x), 1p2e15.6, 5x, ' i, ip, p, p(min) ')
511      173 format (' wall clock:  time = ', a8, ' " hh:mm:ss'
512      &          /'          date = ', a9, ' " yy-mm-dd' )
513
514      181 format (/ number of grid points scanned, kts =', i10
515      &          /' population along the minimum, ktm =', i10
516      &          /' norm of the residual, |g| =', 1p13.5,
517      &          ' (degrees)')
518      182 format (/ model parameter value along the minimum:')
519      183 format (1x, i4, ')', 1p15.5, ', for:', i5, ', (z)',
520      &          a1, ' " boundary')
521      184 format (1x, i4, ')', 1p15.5, ', for:', i5, ', (f)',
522      &          a1, ' " boundary')
523      185 format (1x, i4, ')', 1p15.5, ', for:', i5, ', (p)',
524      &          a1, ' " boundary')
525      186 format (/ Note:    minimum point is near a boundary.')
526
527      end

```

6.2.10 SEEK01.FOR

```

1      subroutine seek01
2      c      -----
3      c      Find a single set of model parameters (z,f,p)
4      c      which minimizes the sum of least-squares error residuals
5      c      to the set of ellipsometric equations governing experiment.
6      c      Method of solution:   damped least-squares analysis.
7      c      -----
8      include 'iounit.'
9      include 'defnit.'
10     include 'filmmm.'
11     include 'xprmnt.'
12     include 'arrays.'           ! aa,bb,xx
13     include 'wstack.'           ! p,u,v,w,xw,se, aat,aats
14     include 'handyy.'           ! pi
15
16     logical    first, jump
17
18     raddeg = 180.0 /pi           ! degrees/radian
19     llnorm = .true.             ! ASMBL, renormalize g
20     call asmb1                   ! ia,ja,aa,bb
21     call norm (meqns, bb, bn, 1) ! residual
22
23     if (bn .eq. 0.0) return
24     bn1 = bn                     ! initial
25     bn2 = bn                     ! last
26     loop = 0
27     niter = mvary*4              ! number of iterations
28     write (iout,111)
29     write (iout,112) loop, bn
30
31     1 itry = 0                   ! stepsize reductions
32     loop = loop+1                ! iterations
33     do i=1,mvary                 ! initialize Newton step
34         xx(i) = 0.0
35     end do
36     call scaljj (meqns,mvary,ia,ja,aa,xx, aats,w,2) ! scale columns, A
37     call cgn1   (meqns,mvary,ia,ja,aa,bb,xx,
38     &           niter,      u,v,w,  xw,se)
39     do i=1,mvary                 ! account for scaling
40         xx(i) = xx(i)/aats(i)    ! columns in SCALJJ
41         se(i) = se(i)/aats(i)
42     end do
43
44     2 do i=1,mvary                ! update
45         j = iptu(i)
46         h = xx(i)*0.4             ! step
47         s = se(i)*0.4             ! estimated standard deviation
48
49         if (j .le. mfilmz) then    ! z, thicknesses
50             f = widths(j)         ! value

```

```

51         g = uwidth(j)                                ! uncertainty
52 c*       write (iout,131) i,f,h,j
53         ha = amax1 (s, f*0.2, 0.05)                   ! upper bound
54         ha = amin1 (g, abs (h), ha)                   ! lower bound
55         if (h.lt.0.0) ha=-ha
56         aat(i) = f                                     ! retain
57         widths(j) = amax1 (0.0, f+ha)                 ! constraint
58     .else if (j .le. mfilmz+mlmnts) then               ! volume fractions
59         j = j-mfilmz
60         f = fflmnt(j)                                ! value
61         g = uflmnt(j)                                ! uncertainty
62 c*       write (iout,132) i,f,h,j
63         ha = amax1 (s, abs (f*0.2), 0.01)             ! upper bound
64         ha = amin1 (g, abs (h), ha)                   ! lower bound
65         if (h.lt.0.0) ha=-ha
66         aat(i) = f                                     ! retain
67         fflmnt(j) = f+ha
68     .else                                              ! parameters
69         j = j-mfilmz-mlmnts
70         f = rrparm(j)                                ! value
71         g = urparm(j)                                ! uncertainty
72 c*       write (iout,133) i,f,h,j
73         ha = amax1 (s, abs (f*0.2))                   ! upper bound
74         ha = amin1 (g, abs (h), ha)                   ! lower bound
75         if (h.lt.0.0) ha=-ha
76         aat(i) = f                                     ! retain
77         rrparm(j) = f+ha
78     .end if
79 .end do
80
81     jump = .false.                                    ! escape switch
82
83     3 do m=1,mmixtr                                    ! algebraic constraint
84         mvlmn = mvlmnt(m)
85         if (mvlmn.ne.0) then                            ! something varies
86             mmlmn = mmlmnt(m)
87             kk = kklmnt(m)
88             j = mfilmz+kk+1
89             if (iptw(j).ne.-1) then                    ! utilized
90                 fu = 0.0
91                 fv = 0.0
92                 first = .true.
93                 do lmn=1,mmlmn
94                     kk = kk+1
95                     if (lflmnt(kk).eq.1) then .! vary
96                         if (first) then
97                             first = .false.
98                             kk1 = kk
99                         .else
100                             fv = fv+fvlmnt(kk)
101                         .end if
102                     .else
103                         fu = fu+fvlmnt(kk)

```



```

104             end if
105             end do      ! volume fractions
106             fflmnt(kk1) = 1.0-fu-fv      ! constraint
107             end if      ! utilized
108             end if      ! vary
109         end do          ! mixture
110
111         if (jump) goto 6      ! escape
112
113         call asmb1            ! ia,ja,aa,bb
114         call norm (meqns, bb, bn, 1)    ! residual
115         total = bn /bn1        ! total reduction
116         relat = bn /bn2        ! relative reduction
117
118         if (total .le. 1.E-5) then      ! convergence
119             bn2 = bn                    ! retain
120             goto 5                      ! escape
121         end if
122
123         if (relat .le. 0.999) then      ! converging
124             bn2 = bn                    ! retain
125             goto 4                      ! iterate
126         end if
127
128         do i=1,mvary                  ! reset
129             j = iptu(i)
130             if (j .le. mfilmz) then
131                 widths(j) = aat(i)
132             else if (j .le. mfilmz+mlmnts) then
133                 j = j-mfilmz
134                 fflmnt(j) = aat(i)
135             else
136                 j = j-mfilmz-mlmnts
137                 rrparm(j) = aat(i)
138             end if
139         end do
140
141         if (itry.lt.3) then            ! try again
142             itry = itry+1
143             do i=1,mvary
144                 xx(i) = xx(i)*0.5      ! reduce stepsize
145             end do
146             goto 2
147         end if
148
149         if (loop .le. 3) then          ! convenience
150             write (iout,114)
151             if (relat .le. 1.0) then    ! marginal
152                 write (iout,115)
153             else                        ! divergence
154                 write (iout,116)
155             end if
156         end if

```

```

157      jump = .true.                ! escape
158      goto 3                      ! constraint
159
160      4 write (iout,113) loop, relat, total, bn
161      goto 1
162      5 write (iout,113) loop, relat, total, bn
163      6 continue
164
165 c      -----
166 c      Output results of iterations involving least-squares.
167
168      write (iout,121)                ! results
169      do i=1,mvary
170          j = iptu(i)
171          if (j .le. mfilmz) then      ! widths
172              write (iout,122) i, widths(j), se(i), j
173          else if (j .le. mfilmz+mlmnts) then ! fractions
174              j = j-mfilmz
175              write (iout,123) i, fflmnt(j), se(i), j
176          else                        ! parameters
177              j = j-mfilmz-mlmnts
178              write (iout,124) i, rrparm(j), se(i), j
179          end if
180      end do
181      write (iout,125) bn1, bn2        ! compare
182
183 c      -----
184      call corlat                    ! correlation matrix
185      call scato1 (3)                ! plot deviations of fit
186      return
187
188      111 format (' seek:  loop,      ratio of reduction,      |g|'
189      &          '/'              (rel)      (total)      ')
190      112 format ( 8x, i5, 24x, 1p1e12.3)
191      113 format ( 8x, i5,      1p3e12.3)
192      114 format ( 8x, 'stepsize reduction attempted.')
193      115 format ( 8x, '... slow convergence.      ')
194      116 format ( 8x, '... divergence.      ')
195
196      121 format (' model parameter value along the minimum:')
197      122 format (5x, i5, ')', f15.4, f10.5, ', for:', i5, ' ^ (z,zu)')
198      123 format (5x, i5, ')', f15.4, f10.5, ', for:', i5, ' ^ (f,fu)')
199      124 format (5x, i5, ')', f15.4, f10.5, ', for:', i5, ' ^ (p,pu)')
200      125 format (' initial |g| =', 1p1e13.5,
201      &          '/'      final |g| =',      e13.5)
202
203      131 format (20x, i5, ')', 1p2e15.5, ', for:', i5, ' ^ (z,dz)')
204      132 format (20x, i5, ')', 1p2e15.5, ', for:', i5, ' ^ (f,df)')
205      133 format (20x, i5, ')', 1p2e15.5, ', for:', i5, ' ^ (p,dp)')
206
207      end

```

6.2.11 SEEKO2.FOR

```

1      subroutine seeko2
2      c      -----
3      c      Find a single set of model parameters (z,f,p)
4      c      which minimizes the sum of least-squares error residuals
5      c      to the set of ellipsometric equations governing experiment.
6      c      Method of solution:   damped least-squares analysis.
7      c      -----
8      include 'iounit.'
9      include 'defnit.'
10     include 'filmmm.'
11     include 'xprmnt.'
12     include 'arrays.'           ! aa,bb,xx
13     include 'wstack.'          ! p,u,v,w,xw,se, aat,aats
14     include 'nesto1.'          ! ppp1, ppp2, ppp3
15     include 'handyy.'          ! pi
16
17     logical   first, jump
18
19     raddeg = 180.0 /pi
20     llnorm = .true.             ! ASMBL, renormalize g
21     call asmb1                  ! ia,ja,aa,bb
22     call norm (meqns, bb, bn, 1) ! residual
23
24     if (bn .eq. 0.0) return
25     bn1 = bn                    ! initial
26     bn2 = bn                    ! last
27     loop = 0
28     niter = mvary*4              ! number of iterations
29     c      write (iout,111)
30     c      write (iout,112) loop, bn
31
32     1 itry = 0                  ! stepsize reductions
33     loop = loop+1               ! iterations
34     do i=1,mvary                ! initialize Newton step
35         xx(i) = 0.0
36     end do
37     call scaljj (meqns,mvary,ia,ja,aa,xx, aats,w,2) ! scale columns, A
38     call cgn1   (meqns,mvary,ia,ja,aa,bb,xx,
39     &           niter,      u,v,w,  xw,se)
40     do i=1,mvary                ! account for scaling
41         xx(i) = xx(i)/aats(i)   ! columns in SCALJJ
42         se(i) = se(i)/aats(i)
43     end do
44
45     2 do i=1,mvary               ! update
46         j = iptu(i)
47         h = xx(i)*0.4           ! step
48         s = se(i)*0.4           ! estimated standard deviation
49
50     if (j .le. mfilmz) then      ! z, thicknesses

```

```

51         f = widths(j)                                ! value
52         g = uwidth(j)                                ! uncertainty
53 c*        write (iout,131) i,f,h,j
54         ha = amax1 (s, f*0.2, 0.05)                  ! upper bound
55         ha = amin1 (g, abs (h), ha, ppp3(i))         ! lower bound
56         if (h.lt.0.0) ha=-ha
57         aat(i) = f                                    ! retain
58         widths(j) = amax1 (0.0, f+ha)                ! constraint
59
60         if (widths(j) .lt. ppp1(i)) then              ! bounds
61             widths(j) = ppp1(i)
62         else if (widths(j) .gt. ppp2(i)) then
63             widths(j) = ppp2(i)
64         end if
65
66     else if (j .le. mfilmz+mlmnts) then                ! volume fractions
67         j = j-mfilmz
68         f = fflmnt(j)                                ! value
69         g = uflmnt(j)                                ! uncertainty
70 c*        write (iout,132) i,f,h,j
71         ha = amax1 (s, abs (f*0.2), 0.01)            ! upper bound
72         ha = amin1 (g, abs (h), ha, ppp3(i))         ! lower bound
73         if (h.lt.0.0) ha=-ha
74         aat(i) = f                                    ! retain
75         fflmnt(j) = f+ha
76
77         if (fflmnt(j) .lt. ppp1(i)) then              ! bounds
78             fflmnt(j) = ppp1(i)
79         else if (fflmnt(j) .gt. ppp2(i)) then
80             fflmnt(j) = ppp2(i)
81         end if
82
83     else                                              ! parameters
84         j = j-mfilmz-mlmnts
85         f = rrparm(j)                                ! value
86         g = urparm(j)                                ! uncertainty
87 c*        write (iout,133) i,f,h,j
88         ha = amax1 (s, abs (f*0.2))                  ! upper bound
89         ha = amin1 (g, abs (h), ha, ppp3(i))         ! lower bound
90         if (h.lt.0.0) ha=-ha
91         aat(i) = f                                    ! retain
92         rrparm(j) = f+ha
93
94         if (rrparm(j) .lt. ppp1(i)) then              ! bounds
95             rrparm(j) = ppp1(i)
96         else if (rrparm(j) .gt. ppp2(i)) then
97             rrparm(j) = ppp2(i)
98         end if
99
100     end if      ! z,f,p
101 end do          ! vary
102
103 jump = .false.                                ! escape switch

```

```

104
105      3 do m=1,mmixtr                                ! algebraic constraint
106          mvlmn = mvlmnt(m)
107          if (mvlmn.ne.0) then                        ! something varies
108              mmlmn = mmlmnt(m)
109              kk = kklmnt(m)
110              j = mfilmz+kk+1
111              if (iptw(j).ne.-1) then                ! utilized
112                  fu = 0.0
113                  fv = 0.0
114                  first = .true.
115                  do lmn=1,mmlmn
116                      kk = kk+1
117                      if (lflmnt(kk).eq.1) then      ! vary
118                          if (first) then
119                              first = .false.
120                              kk1 = kk
121                          else
122                              fv = fv+fllmnt(kk)
123                          end if
124                      else                             ! froz
125                          fu = fu+fllmnt(kk)
126                      end if
127                  end do                               ! volume fractions
128                  fllmnt(kk1) = 1.0-fu-fv            ! constraint
129              end if                                  ! utilized
130          end if                                      ! vary
131      end do                                          ! mixture
132
133      if (jump) goto 6                                ! escape
134
135      call asmb1                                       ! ia,ja,aa,bb
136      call norm (meqns, bb, bn, 1)                   ! residual
137      total = bn /bn1                                ! total reduction
138      relat = bn /bn2                                ! relative reduction
139
140      if (total .le. 1.E-5) then                      ! convergence
141          bn2 = bn                                    ! retain
142          goto 5                                       ! escape
143      end if
144
145      if (relat .le. 0.999) then                      ! converging
146          bn2 = bn                                    ! retain
147          goto 4                                       ! iterate
148      end if
149
150      do i=1,mvary                                    ! reset
151          j = iptu(i)
152          if (j .le. mfilmz) then
153              widths(j) = aat(i)
154          else if (j .le. mfilmz+mlmnts) then
155              j = j-mfilmz
156              fllmnt(j) = aat(i)

```



```

157         else
158             j = j-mfilmz-mlmnts
159             rrparm(j) = aat(i)
160         end if
161     end do
162
163     if (itry.lt.3) then                                ! try again
164         itry = itry+1
165         do i=1,mvary
166             xx(i) = xx(i)*0.5                            ! reduce stepsize
167         end do
168         goto 2
169     end if
170
171 c     if (loop .le. 3) then                                ! convenience
172 c         write (iout,114)
173 c         if (relat .le. 1.0) then                            ! marginal
174 c             write (iout,115)
175 c         else                                                ! divergence
176 c             write (iout,116)
177 c         end if
178 c     end if
179     jump = .true.                                           ! escape
180     goto 3                                                  ! constraint
181
182 4 continue
183 c     write (iout,113) loop, relat, total, bn
184 c     goto 1
185 5 continue
186 c     write (iout,113) loop, relat, total, bn
187 6 continue
188
189 c     -----
190 c     Output results of iterations involving least-squares.
191
192 c     write (iout,121)                                ! results
193 c     do i=1,mvary
194 c         j = iptu(i)
195 c         if (j .le. mfilmz) then                            ! widths
196 c             write (iout,122) i, widths(j), se(i), j
197 c         else if (j .le. mfilmz+mlmnts) then                ! fractions
198 c             j = j-mfilmz
199 c             write (iout,123) i, flmnt(j), se(i), j
200 c         else                                                ! parameters
201 c             j = j-mfilmz-mlmnts
202 c             write (iout,124) i, rrparm(j), se(i), j
203 c         end if
204 c     end do
205 c     write (iout,125) bn1, bn2                                ! compare
206
207 c     -----
208 c     call corlat                                ! correlation matrix
209 c     call scato1 (3)                            ! plot deviations of fit

```

```

210
211      return
212
213      111 format (/ ' seek:   loop,      ratio of reduction,      |g| '
214      &          /'              (rel)        (total)          ' )
215      112 format (      8x, i5, 24x, 1p1e12.3)
216      113 format (      8x, i5,          1p3e12.3)
217      114 format (      8x, 'stepsize reduction attempted.')
218      115 format (      8x, '... slow convergence.          ' )
219      116 format (      8x, '... divergence.                  ' )
220
221      121 format (/ ' model parameter value along the minimum:')
222      122 format (5x, i5, ' ', f15.4, f10.5, ' ', for:', i5, ' - (z,zu)')
223      123 format (5x, i5, ' ', f15.4, f10.5, ' ', for:', i5, ' - (f,fu)')
224      124 format (5x, i5, ' ', f15.4, f10.5, ' ', for:', i5, ' - (p,pu)')
225      125 format (/ ' initial |g| =', 1p1e13.5,
226      &          /'   final |g| =',    e13.5)
227
228      131 format (20x, i5, ' ', 1p2e15.5, ' ', for:', i5, ' - (z,dz)')
229      132 format (20x, i5, ' ', 1p2e15.5, ' ', for:', i5, ' - (f,df)')
230      133 format (20x, i5, ' ', 1p2e15.5, ' ', for:', i5, ' - (p,dp)')
231
232      end

```

6.2.12 ASMBL.FOR

```

1      subroutine asmb1
2      include 'iounit.'
3      include 'defnit.'
4      include 'filmmn.'
5      include 'xprmnt.'
6      include 'arrayd.'
7      include 'arrays.'
8      include 'filmss.'
9      include 'abcdef.'
10     include 'handyy.'          ! pi
11
12     logical      first, firstv
13
14
15     mmm = mfilmz+mlmnts+mrpars
16     do m=1,mmm                ! local, column in a row of: aa
17         if (iptw(m).ne.-1) then ! utilized, retain info from ARRANG
18             iptw(m) = 0        ! global ---> local into: aa
19         end if
20         iptx(m) = 0            ! local ---> global into: iptw
21     end do
22
23     ia(1) = 1
24     ii = 1                    ! IA
25     jj = 0                    ! JA
26     ize = 0                   ! (z,e),sample
27     ias = 0                   ! ambient,sample
28     iras = 0                  ! repeat,ambient,sample
29     ixpts = 0                 ! expt,repeat,ambient,sample
30
31     do is=1,msampl
32         mfilm = mmfilm(is)    ! FILMSS
33         mfilms = mfilm+1      ! films/substrate
34         mfilma = mfilm+2      ! ambient/films/substrate
35         mzs = mfilm*2+1       ! (z,e),(e)
36         mv = 0                ! local, unique, vary
37
38         do m=1,mfilms
39             if (m.ne.mfilms) then ! films
40                 ize = ize+1      ! widths
41                 iwidth = iifilm(ize)
42                 zzz(m) = widths(iwidth) ! FILMSS
43                 if (lwidth(iwidth).eq.1) then ! vary
44                     j = iwidth
45                     if (iptw(j).eq.0) then ! unique, compress
46                         mv = mv+1 ! local
47                         iptw(j) = mv
48                         iptx(mv) = j
49                         jj = jj+1 ! within row A
50                         ja(jj) = iptv(j) ! column, global

```

```

51         end if
52     end if
53 end if
54  ize = ize+1                                ! films/substrate
55  imixtr = iifilm(ize)                        ! mixture
56
57  mixflm(m) = imixtr                          ! initialize
58
59  mvlmn = mvlmnt(imixtr)                      ! vary
60  if (mvlmn.ne.0) then                        ! fraction
61      first = .true.                          ! constraint, 1=u+v
62      mmlmn = mmlmnt(imixtr)                  ! quantity
63      kk = kklmnt(imixtr)                     ! offset
64      do lmn=1,mmlmn
65          kk = kk+1                            ! monotonic
66          if (lflmnt(kk).eq.1) then            ! vary
67              j = mfilmz+kk                    ! global
68              if (first) then                  ! constraint on: dv(1)
69                  first = .false.
70              else if (iptw(j).eq.0) then
71                  mv = mv+1                    ! local unique
72                  iptw(j) = mv
73                  iptx(mv) = j
74                  jj = jj+1                    ! along a row within A
75                  ja(jj) = iptv(j)             ! column
76              end if
77          end if
78      end do
79  end if
80
81  mvpar = mvparm(imixtr)                      ! vary
82  if (mvpar.ne.0) then                        ! parameter
83      mrpar = mrparm(imixtr)                  ! quantity
84      kr = krparm(imixtr)                     ! offset
85      do irp=1,mrpar
86          kr = kr+1                            ! offset
87          ip = jrparm(kr)                      ! specify index
88          if (lrparm(ip).eq.1) then            ! vary
89              j = mfilmz+mlmnts+ip             ! global, unique
90              if (iptw(j).eq.0) then            ! unique
91                  mv = mv+1                    ! local, compress, aa
92                  iptw(j) = mv
93                  iptx(mv) = j
94                  jj = jj+1
95                  ja(jj) = iptv(j)             ! column
96              end if
97          end if
98      end do
99  end if
100 end do
101
102  mvsav = mv                                  ! convenience
103  jjsav = jj

```

```

104
105      mbien = mmbent(is)                ! quantity
106      do mbn=1,mbien                    ! ambients
107          ias = ias+1
108          mrpeat = mmpeat(ias)
109          imbien = iibent(ias)           ! specify ambient
110          imixtr = mixmbn(imbien)        ! mixture used as ambient
111
112          mixflm(mfilms+1) = imixtr      ! mixture used as ambient
113          mv = mvsav
114          jj = jjsav
115
116          mvlmn = mvlmnt(imixtr)         ! vary
117          if (mvlmn.ne.0) then           ! fractions
118              first = .true.
119              mmlmn = mmlmnt(imixtr)
120              kk = kklmnt(imixtr)        ! offset
121              do lmn=1,mmlmn             ! fractions
122                  kk = kk+1
123                  if (lflmnt(kk).eq.1) then ! vary
124                      j = mfilmz+kk
125                      if (first) then     ! constraint
126                          first = .false.
127                      else if (iptw(j).eq.0) then
128                          mv = mv+1      ! local, compress
129                          iptw(j) = mv
130                          iptx(mv) = j
131                          jj = jj+1      ! along a row in A
132                          ja(jj) = iptv(j) ! column
133                      end if
134                  end if ! vary
135              end do ! fractions
136          end if ! something varies
137
138          mvpar = mvparm(imixtr)         ! vary
139          if (mvpar.ne.0) then           ! parameters
140              mrpar = mrparm(imixtr)
141              kr = krparm(imixtr)        ! offset
142              do irp=1,mrpar
143                  kr = kr+1
144                  ip = jrparm(kr)        ! specify index
145                  if (lrparm(ip).eq.1) then
146                      j = mfilmz+mlmnts+ip
147                      if (iptw(j).eq.0) then ! unique
148                          mv = mv+1
149                          iptw(j) = mv
150                          iptx(mv) = j
151                          jj = jj+1
152                          ja(jj) = iptv(j)
153                      end if
154                  end if
155              end do
156          end if

```



```

157
158      mm = mmixtr+imbien      ! offset, ambient
159      mvpar = mvparm(mm)      ! vary
160      if (mvpar.ne.0) then    ! parameter
161          mrpar = mrparm(mm)  ! quantity
162          kr = krparm(mm)     ! offset
163          do irp=1,mrpar
164              kr = kr+1        ! offset
165              ip = jrparm(kr)  ! specify index
166              if (lrparm(ip).eq.1) then ! vary
167                  j = mfilmz+mlmnts+ip ! global
168                  if (iptw(j).eq.0) then ! unique
169                      mv = mv+1        ! local, compress, aa
170                      iptw(j) = mv
171                      iptx(mv) = j
172                      jj = jj+1
173                      ja(jj) = iptv(j)
174                  end if
175              end if
176          end do
177      end if      ! something varies
178
179      if (mv.eq.0) then      ! something should vary
180          write (iout,102) is,mbn
181          stop
182      end if
183
184      mvvari = mv            ! local quantity
185      firstv = .true.        ! yet need row: delta
186
187      do irpeat=1,mrpeat    ! repeats
188          iras = iras+1
189          mexpt = mmexpt(iras)
190
191          needs = jj + mv + mv*(mexpt-1)*2
192          if (nnjaaa .lt. needs) then
193              write (iout,103) needs
194              stop
195          end if
196
197          do ixpt=1,mexpt    ! measurements
198              ixpts = ixpts+1
199
200              wavln1 = wavlns(ixpts) ! nano-meters
201              wavln2 = wavlnu(ixpts)
202              angle1 = angles(ixpts) ! radians
203              angle2 = angleu(ixpts)
204              psi1 = psiis(ixpts) ! radians
205              psi2 = psiuu(ixpts)
206              delta1 = deltas(ixpts) ! radians
207              delta2 = deltau(ixpts)
208
209              do m=1,mfilma ! initialize, indicate

```

```

210         i = mixflm(m)
211         firstx(i) = .true.      !    need of evaluation
212     end do
213
214 c         Discern:    dielectric functions (z)
215
216         imixtr = mixmbn(imbien)          ! ambient
217         firstx(imixtr) = .false.
218         call diefcn (imbien, imixtr, angle1, wavln1,
219 &             dielec( imixtr), dielew( imixtr),
220 &             dielff(1,imixtr),
221 &             dielpp(1,imixtr), dielpa(1,imixtr))
222
223         izz = izz-mzs                    ! reset pointer
224     do m=1,mfilms
225         if (m.ne.mfilms) then            ! skip widths
226             izz = izz+1
227         end if
228         izz = izz+1
229         imixtr = iifilm(izz)
230         if (firstx(imixtr)) then          ! first
231             firstx(imixtr) = .false.
232             call diefcn (imbien, imixtr,
233 &                 angle1, wavln1,
234 &                 dielec( imixtr), dielew( imixtr),
235 &                 dielff(1,imixtr),
236 &                 dielpp(1,imixtr), dielpa(1,imixtr))
237         end if
238         die(m) = dielec(imixtr)
239     end do                                ! films
240
241     isampl = is
242     izsmpl = izz-mzs                      ! reset index
243     call scattr (wavln1, angle1,
244 &         isampl, izsmpl, imbien, mvari)
245
246     bb(ii ) = psi1 - b(1)                 ! psi
247 c*     bb(ii+1) = delta1 - b(2)            ! delta
248     call differ (delta1, b(2), diff)
249     bb(ii+1) = diff
250
251     ia(ii+1) = ia(ii )+mv                 ! psi
252     ia(ii+2) = ia(ii+1)+mv                ! delta
253
254     if (firstv) then                      ! psi (row A) already completed
255         firstv = .false.
256         do j=1,mv                         ! unique
257             jj = jj+1
258             ja(jj) = ja(jj-mv)            ! delta
259         end do
260     else
261         do j=1,mv
262             jj = jj+1

```

```

263             ja(jj ) = ja(jj-mv)           ! psi
264             ja(jj+mv) = ja(jj )           ! delta
265             end do
266             jj = jj+mv                       ! end of second row
267         end if
268
269         jv = 0
270         j1 = ia(ii )
271         j2 = ia(ii+1)-1
272         do j=j1,j2                           ! initialize
273             aa(j ) = a(jv+1)                 ! psi
274             aa(j+mv) = a(jv+2)              ! delta
275             jv = jv+2
276         end do
277
278 c         Renormalize the rows in the Jacobian matrix
279
280         if (llnorm) then
281             bb(ii ) = bb(ii )/psi2           ! psi
282             bb(ii+1) = bb(ii+1)/delta2       ! delta
283             do j=j1,j2
284                 aa(j ) = aa(j )/psi2        ! psi
285                 aa(j+mv) = aa(j+mv)/delta2  ! delta
286             end do
287         end if
288
289         ii = ii+2
290     end do      ! measurements
291 end do        ! repeats
292
293     if (mv.gt.mvsav) then      ! reset unique-ness
294         mv1 = mvsav+1
295         do i=mv1,mv
296             j = iptx(i)        ! point to:   iptw
297             iptw(j) = 0        ! unique-ness
298             iptx(i) = 0
299         end do
300     end if
301 end do      ! ambients
302
303     if (mvsav.ne.0) then      ! reset unique-ness
304         do i=1,mvsav
305             j = iptx(i)        ! point to:   iptw
306             iptw(j) = 0        ! unique-ness
307             iptx(i) = 0
308         end do
309     end if
310 end do      ! sample
311 meqns = ii-1
312
313 if (jj .ne. ia(ii)-1) then
314     write (iout,104) ii, jj, ia(ii)
315     stop

```

```

316         end if
317
318         return
319
320     102 format (' asmb1, something should vary in the Jacobian,'
321               &      '/' sample=', i2, ', ambient=', i2)
322     103 format (' asmb1, insufficient array allocation for: aa,ja'
323               &      '/' see named common: arrays. '
324               &      '/' update to atleast: ', i10 )
325     104 format (' asmb1, inconsistent formating of sparse matrix,'
326               &      '/' ii = ', i10
327               &      '/' jj = ', i10, ' =/=', i10, ' = ia(ii)-1')
328
329         end

```

6.2.13 ASMBL0.FOR

```

1      subroutine  asmb10                      ! residual only
2      include    'iounit.'
3      include    'defnit.'
4      include    'filmm.'
5      include    'xprmt.'
6      include    'arrayd.'
7      include    'arrays.'
8      include    'filmss.'
9      include    'abcdef.'
10     include    'handyy.'                    ! pi
11
12     logical     first, firstv
13
14     mmm = mfilmz+mlmnts+mrpars
15     do m=1,mmm                                ! local, column in a row of: aa
16         if (iptw(m).ne.-1) then                ! utilized, retain info from ARRANG
17             iptw(m) = 0                        ! global ---> local    into: aa
18         end if
19         iptx(m) = 0                            ! local ---> global    into: iptw
20     end do
21
22     ia(1) = 1
23     ii = 1                                    ! IA
24     jj = 0                                    ! JA
25     ize = 0                                    ! (z,e) ,sample
26     ias = 0                                    ! ambient,sample
27     iras = 0                                  ! repeat,ambient,sample
28     ixpts = 0                                ! expt,repeat,ambient,sample
29
30     do is=1,msampl
31         mfilm = mmfilm(is)                    ! FILMSS
32         mfilms = mfilm+1                      ! films/substrate
33         mfilma = mfilm+2                     ! ambient/films/substrate
34         mzs = mfilm*2+1                      ! (z,e),(e)
35         mv = 0.                              ! local, unique, vary
36
37         do m=1,mfilms
38             if (m.ne.mfilms) then                ! films
39                 ize = ize+1                    ! widths
40                 iwidth = iifilm(ize)
41                 zzz(m) = widths(iwidth)        ! FILMSS
42                 if (lwidth(iwidth).eq.1) then ! vary
43                     j = iwidth
44                     if (iptw(j).eq.0) then      ! unique, compress
45                         mv = mv+1                ! local
46                         iptw(j) = mv
47                         iptx(mv) = j
48                         jj = jj+1                ! within row A
49                         ja(jj) = iptv(j)         ! column, global
50                 end if

```



```

51         end if
52     end if
53     ize = ize+1                                ! films/substrate
54     imixtr = iifilm(ize)                        ! mixture
55
56     mixflm(m) = imixtr                          ! initialize
57
58     mvlmn = mvlmnt(imixtr)                      ! vary
59     if (mvlmn.ne.0) then                        ! fraction
60         first = .true.                          ! constraint, 1=u+v
61         mmlmn = mmlmnt(imixtr)                  ! quantity
62         kk = kklmnt(imixtr)                     ! offset
63         do lmn=1,mmlmn
64             kk = kk+1                            ! monotonic
65             if (lflmnt(kk).eq.1) then            ! vary
66                 j = mfilmz+kk                    ! global
67                 if (first) then                  ! constraint on: dv(1)
68                     first = .false.
69                 else if (iptw(j).eq.0) then
70                     mv = mv+1                    ! local unique
71                     iptw(j) = mv
72                     iptx(mv) = j
73                     jj = jj+1                    ! along a row within A
74                     ja(jj) = iptv(j)             ! column
75                 end if
76             end if                                ! vary
77         end do                                    ! fraction
78     end if                                        ! something varies
79
80     mvpar = mvparm(imixtr)                      ! vary
81     if (mvpar.ne.0) then                        ! parameter
82         mrpar = mrparm(imixtr)                  ! quantity
83         kr = krparm(imixtr)                     ! offset
84         do irp=1,mrpar
85             kr = kr+1                            ! offset
86             ip = jrparm(kr)                      ! specify index
87             if (lrparm(ip).eq.1) then            ! vary
88                 j = mfilmz+mlmnts+ip            ! global, unique
89                 if (iptw(j).eq.0) then            ! unique
90                     mv = mv+1                    ! local, compress, aa
91                     iptw(j) = mv
92                     iptx(mv) = j
93                     jj = jj+1
94                     ja(jj) = iptv(j)             ! column
95                 end if
96             end if                                ! vary
97         end do                                    ! parameters
98     end if                                        ! something varies
99 end do                                            ! mfilms
100
101     mvsav = mv                                    ! convenience
102     jjsav = jj
103

```

```

104      mbien = mmbent(is)                ! quantity
105      do mbn=1,mbien                    ! ambients
106          ias = ias+1
107          mrpeat = mmpeat(ias)
108          imbien = iibent(ias)           ! specify ambient
109          imixtr = mixmbn(imbien)        ! mixture used as ambient
110
111          mixflm(mfilms+1) = imixtr      ! mixture used as ambient
112          mv = mvsav
113          jj = jjsav
114
115          mvlmn = mvlmnt(imixtr)         ! vary
116          if (mvlmn.ne.0) then           ! fractions
117              first = .true.
118              mmlmn = mmlmnt(imixtr)
119              kk = kklmnt(imixtr)        ! offset
120              do lmn=1,mmlmn             ! fractions
121                  kk = kk+1
122                  if (lflmnt(kk).eq.1) then ! vary
123                      j = mfilmz+kk
124                      if (first) then     ! constraint
125                          first = .false.
126                      else if (iptw(j).eq.0) then
127                          mv = mv+1      ! local, compress
128                          iptw(j) = mv
129                          iptx(mv) = j
130                          jj = jj+1      ! along a row in A
131                          ja(jj) = iptv(j) ! column
132                      end if
133                  end if ! vary
134              end do ! fractions
135          end if ! something varies
136
137          mvpar = mvparm(imixtr)         ! vary
138          if (mvpar.ne.0) then           ! parameters
139              mrpar = mrparm(imixtr)
140              kr = krparm(imixtr)        ! offset
141              do irp=1,mrpar
142                  kr = kr+1
143                  ip = jrparm(kr)        ! specify index
144                  if (lrparm(ip).eq.1) then
145                      j = mfilmz+mlmnts+ip
146                      if (iptw(j).eq.0) then ! unique
147                          mv = mv+1
148                          iptw(j) = mv
149                          iptx(mv) = j
150                          jj = jj+1
151                          ja(jj) = iptv(j)
152                      end if
153                  end if
154              end do
155          end if
156

```

```

157      mm = mmixtr+imbien      ! offset, ambient
158      mvpar = mvparm(mm)      ! vary
159      if (mvpar.ne.0) then      ! parameter
160          mrpar = mrparm(mm)    ! quantity
161          kr = krparm(mm)      ! offset
162          do irp=1,mrpar
163              kr = kr+1          ! offset
164              ip = jrparm(kr)    ! specify index
165              if (lrparm(ip).eq.1) then ! vary
166                  j = mfilmz+mlmnts+ip ! global
167                  if (iptw(j).eq.0) then ! unique
168                      mv = mv+1      ! local, compress, aa
169                      iptw(j) = mv
170                      iptx(mv) = j
171                      jj = jj+1
172                      ja(jj) = iptv(j)
173                  end if
174              end if
175          end do
176      end if      ! something varies
177
178      c*      if (mv.eq.0) then      ! something should vary
179      c*          write (iout,102) is,mbn
180      c*          stop
181      c*      end if
182
183      mvvari = mv      ! local quantity
184      firstv = .true.  ! yet need row: delta
185
186      do irpeat=1,mrpeat      ! repeats
187          iras = iras+1
188          mexpt = mmexpt(iras)
189
190      c*          needs = jj + mv + mv*(mexpt-1)*2
191      c*          if (nnjaaa .lt. needs) then
192      c*              write (iout,103) needs
193      c*              stop
194      c*          end if
195
196      do ixpt=1,mexpt      ! measurements
197          ixpts = ixpts+1
198
199          wavln1 = wavlns(ixpts)      ! nano-meters
200          wavln2 = wavlnu(ixpts)
201          angle1 = angles(ixpts)      ! radians
202          angle2 = angleu(ixpts)
203          psi1 = psiiis(ixpts)      ! radians
204          psi2 = psiiiu(ixpts)
205          delta1 = deltas(ixpts)      ! radians
206          delta2 = deltau(ixpts)
207
208          do m=1,mfilma      ! initialize, indicate
209              i = mixflm(m)

```

```

210          firstx(i) = .true.      !    need of evaluation
211      end do
212
213  c      Discern:    dielectric functions (z)
214
215          imixtr = mixmbn(imbien)          ! ambient
216          firstx(imixtr) = .false.
217          call diefcn (imbien, imixtr, angle1, wavln1,
218      &              dielec( imixtr), dielew( imixtr),
219      &              dielff(1,imixtr),
220      &              dielpp(1,imixtr), dielpa(1,imixtr))
221
222          ize = ize-mzs                ! reset pointer
223      do m=1,mfilms
224          if (m.ne.mfilms) then        ! skip widths
225              ize = ize+1
226          end if
227          ize = ize+1
228          imixtr = iifilm(ize)
229          if (firstx(imixtr)) then      ! first
230              firstx(imixtr) = .false.
231              call diefcn (imbien, imixtr,
232      &                  angle1, wavln1,
233      &                  dielec( imixtr), dielew( imixtr),
234      &                  dielff(1,imixtr),
235      &                  dielpp(1,imixtr), dielpa(1,imixtr))
236          end if
237          die(m) = dielec(imixtr)
238      end do                ! films
239
240          isampl = is
241          izsmpl = ize-mzs          ! reset index
242          call scatt0 (wavln1, angle1,
243      &              isampl, izsmpl, imbien, mvari)
244
245          bb(ii ) = psi1 - b(1)      ! psi
246  c*      bb(ii+1) = delta1 - b(2)    ! delta
247          call differ (delta1, b(2), diff)
248          bb(ii+1) = diff
249
250  c*      ia(ii+1) = ia(ii )+mv      ! psi
251  c*      ia(ii+2) = ia(ii+1)+mv     ! delta
252
253  c*      if (firstv) then          ! psi (row A) already completed
254  c*          firstv = .false.
255  c*          do j=1,mv              ! unique
256  c*              jj = jj+1
257  c*              ja(jj) = ja(jj-mv) ! delta
258  c*          end do
259  c*      else
260  c*          do j=1,mv
261  c*              jj = jj+1
262  c*              ja(jj ) = ja(jj-mv) ! psi

```

```

283 c*          ja(jj+mv) = ja(jj  )          ! delta
284 c*          end do
285 c*          jj = jj+mv                      ! end of second row
286 c*          end if
287
288 c*          jv = 0
289 c*          j1 = ia(ii  )
290 c*          j2 = ia(ii+1)-1
291 c*          do j=j1,j2                      ! initialize
292 c*              aa(j  ) = a(jv+1)          ! psi
293 c*              aa(j+mv) = a(jv+2)          ! delta
294 c*              jv = jv+2
295 c*          end do
296
297 c*          Renormalize the rows in the Jacobian matrix
298
299 c*          if (llnorm) then
300 c*              bb(ii  ) = bb(ii  )/psi2      ! psi
301 c*              bb(ii+1) = bb(ii+1)/delta2    ! delta
302 c*              do j=j1,j2
303 c*                  aa(j  ) = aa(j  )/psi2    ! psi
304 c*                  aa(j+mv) = aa(j+mv)/delta2 ! delta
305 c*              end do
306 c*          end if
307
308 c*          ii = ii+2
309 c*          end do          ! measurements
310 c*          end do          ! repeats
311
312 c*          if (mv.gt.mvsav) then      ! reset unique-ness
313 c*              mv1 = mvsav+1
314 c*              do i=mv1,mv
315 c*                  j = iptx(i)          ! point to:   iptw
316 c*                  iptw(j) = 0          ! unique-ness
317 c*                  iptx(i) = 0
318 c*              end do
319 c*          end if
320 c*          end do          ! ambients
321
322 c*          if (mvsav.ne.0) then      ! reset unique-ness
323 c*              do i=1,mvsav
324 c*                  j = iptx(i)          ! point to:   iptw
325 c*                  iptw(j) = 0          ! unique-ness
326 c*                  iptx(i) = 0
327 c*              end do
328 c*          end if
329 c*          end do          ! sample
330 c*          meqns = ii-1
331
332 c*          if (jj .ne. ia(ii)-1) then
333 c*              write (iout,104) ii, jj, ia(ii)
334 c*              stop
335 c*          end if

```



```

316
317     return
318
319     102 format (' asmb10, something should vary in the Jacobian,'
320             &      '/'      sample=', i2, ',      ambient=', i2)
321     103 format (' asmb10, insufficient array allocation for:  aa,ja'
322             &      '/'      see named common:   arrays. '
323             &      '/'      update to atleast: ', i10  )
324     104 format (' asmb10, inconsistent formating of sparse matrix,'
325             &      '/'      ii = ', i10
326             &      '/'      jj = ', i10, ' =/=', i10, ' = ia(ii)-1')
327
328     end

```

6.2.14 ARRANG.FOR

```

1      subroutine arrang                      ! discern global pointers
2      include 'iounit.'
3      include 'defnit.'
4      include 'filmmm.'
5      include 'xprmnt.'
6      include 'arrays.'
7
8      logical first
9
10     c      The sparse matrix format of model parameters involve:
11     c      [z(1), z(2), ..., z(mfilmz)],
12     c      [      f(2), ..., f(mlmnts)]_(mixture first), ...
13     c      [      f(2), ...                ]_(mixture last ),
14     c      [p(1), p(2), ...                ]_(mixture first), ...
15     c      [p(1), ...                      ]_(mixture last ),
16     c      [p(1), ...                      ]_(ambient first), ...
17     c      [p(1), ...                      ]_(ambient last ).
18
19     c      where entities under-going variation are:
20     c      z ^ widths,
21     c      f ^ volume fractions,
22     c      p ^ parameters associated with distinct mixtures,
23     c      p ^ parameters associated with distinct ambient/modulation.
24
25     c      The constraint on volume fractions within each mixture is:
26     c      1=v+u ==> dv(1) = -dv(2)-dv(3)- ...
27
28
29     c      Initialize distinct quantities which may undergo variation.
30
31     mmm = mfilmz+mlmnts+mrpars
32     do m=1,mmm
33         iptw(m) = -1                      ! initialize
34     end do
35
36     c      Discern contiguous-ness of model parameters.
37
38     k = 0                                ! (z,e),(e)
39     ias = 0                              ! ambient,sample
40     do is=1,msampl
41         mfilm = mmfilm(is)
42         mfilms = mfilm+1                  ! films,substrate
43         do m=1,mfilms
44             if (m.ne.mfilms) then        ! widths
45                 k = k+1
46                 iwidth = iifilm(k)
47                 if (lwidth(iwidth).eq.1) then ! vary
48                     iptw(iwidth) = 1
49                 else                      ! froz
50                     iptw(iwidth) = 0

```

```

51         end if
52     end if
53     k = k+1                                ! dielectric function
54     imixtr = iifilm(k)                     ! mixture
55
56     mmlmn = mmlmnt(imixtr)                 ! volume fractions
57     if (mmlmn.ne.0) then                   ! existence
58         kk = kklmnt(imixtr)               ! offset
59         do lmn=1,mmlmn
60             kk = kk+1
61             j = mfilmz+kk
62             if (lflmnt(kk).eq.1) then      ! vary
63                 iptw(j) = 1
64             else                            ! froz
65                 iptw(j) = 0
66             end if
67         end do
68     end if                                ! fractions
69
70     mrpar = mrparm(imixtr)                 ! parameters
71     if (mrpar.ne.0) then                   ! existence
72         kr = krparm(imixtr)               ! offset
73         do irp=1,mrpar
74             kr = kr+1
75             ip = jxparm(kr)
76             j = mfilmz+mlmnts+ip
77             if (lrparm(ip).eq.1) then      ! vary
78                 iptw(j) = 1
79             else                            ! froz
80                 iptw(j) = 0
81             end if
82         end do
83     end if                                ! parameters
84 end do                                    ! films
85
86     mbien = mmbent(is)                     ! quantity
87     do mbn=1,mbien                         ! ambients + modulations
88         ias = ias+1
89         imbien = iibent(ias)               ! specify ambient
90         imixtr = mixmbn(imbien)           ! mixture used as ambient
91
92         mmlmn = mmlmnt(imixtr)             ! volume fractions
93         if (mmlmn.ne.0) then               ! existence
94             kk = kklmnt(imixtr)           ! offset
95             do lmn=1,mmlmn
96                 kk = kk+1
97                 j = mfilmz+kk
98                 if (lflmnt(kk).eq.1) then ! vary
99                     iptw(j) = 1
100                else                            ! froz
101                    iptw(j) = 0
102                end if
103            end do

```

```

104         end if          ! fractions
105
106         mrpar = mrparm(imixtr)          ! parameters
107         if (mrpar.ne.0) then             ! existence
108             kr = krparm(imixtr)          ! offset
109             do i=1,mrpar
110                 kr = kr+1
111                 ip = jrparm(kr)
112                 j = mfilmz+mlmnts+ip
113                 if (lrparm(ip).eq.1) then ! vary
114                     iptw(j) = 1
115                 else                       ! froz
116                     iptw(j) = 0
117                 end if
118             end do
119         end if          ! parameters
120
121         mm = mmixtr+imbien
122         mrpar = mrparm(mm)                ! ambient modulation
123         if (mrpar.ne.0) then               ! existence
124             kr = krparm(mm)                ! offset
125             do i=1,mrpar
126                 kr = kr+1
127                 ip = jrparm(kr)
128                 j = mfilmz+mlmnts+ip
129                 if (lrparm(ip).eq.1) then ! vary
130                     iptw(j) = 1
131                 else                       ! froz
132                     iptw(j) = 0
133                 end if
134             end do
135         end if          ! modulation parameters
136     end do              ! ambients
137 end do                  ! sample
138 c =====
139 c Induce ordering on model parameters, (z,f,p).
140
141     jj = 0              ! index extraneous baggage
142     i = 0               ! vary ~ compress
143     k = 0               ! froz ~ compress
144     if (mfilmz .ne. 0) then
145         do m=1,mfilmz   ! film widths
146             if (iptw(m).eq.1) then ! vary + utilized
147                 i = i+1          ! compress
148                 iptu(i) = m       ! full (vary)
149                 iptv(m) = i       ! vary (full)
150             else if (iptw(m).eq.0) then ! froz + utilized
151                 k = k+1          ! compress
152                 km = nrowss+1-k   ! backwards
153                 iptu(km) = m       ! full (froz)
154                 iptv(m) = km       ! froz (full)
155             else              ! extraneous baggage
156                 jj = jj+1

```

```

157         write (iout,1011) m
158     end if
159 end do
160 end if
161
162 do m=1,mmixtr
163     mmlmn = mmlmnt(m)
164     if (mmlmn.ne.0) then
165         kk = kklmnt(m)
166         j = mfilmz+kk+1
167
168         if (iptw(j).eq.-1) then
169             jj = jj+1
170             write (iout,1012) m
171         else
172             first = .true.
173             do lmn=1,mmlmn
174                 kk = kk+1
175                 j = mfilmz+kk
176                 if (lflmnt(kk).eq.1) then
177                     if (first) then
178                         first = .false.
179                     else
180                         i = i+1
181                         iptu(i) = j
182                         iptv(j) = i
183                     end if
184                 else
185                     k = k+1
186                     km = nrowss+1-k
187                     iptu(km) = j
188                     iptv(j) = km
189                 end if
190             end do
191         end if
192     end if
193 end do
194
195 if (mrpars.ne.0) then
196     j = mfilmz+mlmnts
197     do m=1,mrpars
198         j = j+1
199         if (iptw(j).eq.1) then
200             i = i+1
201             iptu(i) = j
202             iptv(j) = i
203         else if (iptw(j).eq.0) then
204             k = k+1
205             km = nrowss+1-k
206             iptu(km) = j
207             iptv(j) = km
208         else
209             jj = jj+1

```

! volume fractions
! quantity
! existence
! offset
! test extraneous mixture

! extraneous baggage

! utilized
! constraint: 1 = v+u

! offset, monotonic
! distinct, unique
! vary volume fraction
! constraint:
! dv(1)=-dv(2)-dv(3)-...

! compress
! full (vary)
! vary (full)

! froz + utilized
! compress
! backwards
! full (froz)
! froz (full)

! fractions
! utilized
! existence
! mixture

! parameters
! offset

! vary, utilized
! compress
! full (vary)
! vary (full)
! froz, utilized
! compress
! backwards
! full (froz)
! froz (full)
! extraneous


```

210         if (lrparm(m).eq.1) then           !      vary
211             write (iout,1013) m
212         else                                 !      froz
213             write (iout,1014) m
214         end if
215     end if
216 end do           ! parameters
217 end if           ! existence
218
219 c -----
220 c This is not necessary, because we test:   iptw(j)/= -1,
221 c are set to zero from within:
222 c     ASMBL, SCAT01, SCAT02.
223
224 if (jj.ne.0) stop
225 c -----
226
227 mvary = i           ! compress
228 mfroz = k           ! compress
229
230 return
231 1011 format (' note:   extraneous      width ', i4)
232 1012 format (' note:   extraneous  mixture ', i4, ', (fraction)')
233 1013 format (' note:   extraneous parameter ', i4, ', (vary)'   )
234 1014 format (' note:   extraneous parameter ', i4, ', (froz)'   )
235 end

```

6.2.15 SCATTR.FOR

```

1      subroutine scattr (wavlen, anglei, isampl, izsmpl, imbien, mvari)
2
3      include 'iounit.'
4      include 'defnit.'
5      include 'filmmm.'
6      include 'arrayd.'
7      include 'arrays.'
8      include 'filmss.'          ! z,e
9      include 'rstack.'         ! R, dR
10     include 'abcdef.'         ! a,b,c ----> output results
11     include 'handyy.'         ! pi,cccc,wavlev
12
13     complex  dRssum(nrowsf), dRpsum(nrowsf), dRsw,dRpw
14     complex  dedf, dedff, dedp
15     logical  first
16
17
18     imixtr = mixmbn(imbien)          ! mixture used as ambient
19     air = sqrt (real (dielec (imixtr))) ! refractive index, FILMSS
20
21     if (wavlen .lt. 0.0) then          ! wavelength, nm
22         qqq = -(pi+pi)/wavlen         !      inverse nm
23     else                               ! energy, eV
24         qqq = (pi+pi)*wavlen/wavlev   !      inverse nm
25     end if
26
27     call forwrd (qqq, anglei)
28
29     sx = real (Rs)
30     sy = aimag (Rs)
31     px = real (Rp)
32     py = aimag (Rp)
33     call polar (sx,sy,sr,sa,1)
34     call polar (px,py,pr,pa,1)
35
36     if (sr.eq.0.0) then
37         if (pr.eq.0.0) then
38             psi = 0.0
39         else
40             psi = 0.5*pi
41         end if
42     else if (pr.eq.0.0) then          ! sr > 0.0
43         psi = 0.0
44     else if (pr.le.sr) then
45         psi = atan (pr/sr)
46     else
47         psi = 0.5*pi - atan(sr/pr)
48     end if
49
50     delta = pa-sa

```

```

51      1 if (delta.lt.0.0) then
52          delta = delta+2.0
53          goto 1
54      else if (delta.ge.2.0) then
55          delta = delta-2.0
56          goto 1
57      end if
58      delta = delta*pi
59
60      b(1) = psi                ! radians
61      b(2) = delta              ! radians
62
63  c      -----
64  c      Note:    q ~ radian/nanometer,      dR/dq ~ nanometer/radian
65  c              q = w/c = (2*pi/hc) * [energy (eV)]
66  c              dq/d(energy (eV)) ~ radian/[nanometer-(eV)]
67
68      hcp = (pi+pi)/wavlev      ! dq/d(energy) ~ (2*pi/hc)
69      dRsw = dRs*cmplx (hcp, 0.0) ! inverse (eV)
70      dRpw = dRp*cmplx (hcp, 0.0)
71  c      =====
72      if (mvari.eq.0) goto 2
73
74      do i=1,mvari              ! remove degeneracy, compress
75          dRssum(i) = cmplx (0.0, 0.0)
76          dRpsum(i) = cmplx (0.0, 0.0)
77      end do
78
79      mm = mmixtr+imbien        ! offset, ambient
80      iv = 0                    ! (z,e), (e)
81      izs = izsmpl
82      mzs = mfilm*2+1          ! (z,e), (e)
83      mfilms = mfilm+1
84      do m=1,mfilms            ! films/substrate
85          if (m.ne.mfilms) then
86              iv = iv+1
87              izs = izs+1
88              iwidth = iifilm(izs)
89              if (lwidth(iwidth).eq.1) then
90                  j = iwidth
91                  mv = iptw(j)
92                  dRssum(mv) = dRssum(mv) + dRs(iv)
93                  dRpsum(mv) = dRpsum(mv) + dRp(iv)
94              end if
95          end if
96          iv = iv+1
97          izs = izs+1
98          imixtr = iifilm(izs)
99
100         mmlmn = mmlmnt(imixtr) ! fractions
101         mvlmn = mvlmnt(imixtr)
102         if (mvlmn.ne.0) then    ! vary
103             kk = kklmnt(imixtr) ! offset

```

```

104         first = .true.
105         do lmn=1,mmlmn
106             kk = kk+1
107             if (lflmnt(kk).eq.1) then          ! vary
108                 j = mfilmz+kk
109                 if (first) then                ! constraint
110                     first = .false.
111                     dedff = dielff(lmn,imixtr)
112                 else
113                     mv = iptw(j)
114                     dedf = dielff(lmn,imixtr) - dedff
115                     dRssum(mv) = dRssum(mv) + dRs(iv)*dedf
116                     dRpsum(mv) = dRpsum(mv) + dRp(iv)*dedf
117                 end if
118             end if          ! vary
119         end do            ! fraction
120     end if                ! existence
121
122     if (mmlmn.ne.0) then          ! dR/dw = (dR/de)*(de/dw)
123         dRsw = dRsw + dRs(iv)*dielew(imixtr)
124         dRpw = dRpw + dRp(iv)*dielew(imixtr)
125     end if
126
127     mrpar = mrparm(imixtr)          ! mixture parameters
128     mvpar = mvparm(imixtr)
129     if (mvpar.ne.0) then            ! vary
130         kr = krparm(imixtr)        ! offset
131         do irp=1,mrpar
132             kr = kr+1
133             ip = jrparm(kr)
134             if (lrparm(ip).eq.1) then
135                 j = mfilmz+mlmnts+ip
136                 mv = iptw(j)
137                 dedp = dielpp(irp,imixtr)
138                 dRssum(mv) = dRssum(mv) + dRs(iv)*dedp
139                 dRpsum(mv) = dRpsum(mv) + dRp(iv)*dedp
140             end if          ! vary
141         end do            ! parameters
142     end if                ! existence
143
144 c      Here, we assume that ambient mixture does NOT vary, but
145 c      parameters associated with an external modulation MAY vary,
146 c      i.e., whenever they modify the dielectric properties of a
147 c      layer within the sample.
148
149     mrpar = mrparm(mm)              ! ambient parameters
150     mvpar = mvparm(mm)
151     if (mvpar.ne.0) then            ! vary
152         kr = krparm(mm)            ! offset
153         do irp=1,mrpar
154             kr = kr+1
155             ip = jrparm(kr)
156             if (lrparm(ip).eq.1) then

```

```

157          j = mfilmz+mlmnts+ip
158          mv = iptw(j)
159          dedp = dielpa(irp,imixtr)
160          dRssum(mv) = dRssum(mv) + dRs(iv)*dedp
161          dRpsum(mv) = dRpsum(mv) + dRp(iv)*dedp
162          end if          ! vary
163          end do          ! parameters
164          end if          ! existence
165
166          end do          ! films
167 c      =====
168
169          k = 0
170          do i=1,mvari          ! Jacobian
171              sxd = real (dRssum(i))
172              syd = aimag (dRssum(i))
173              pxd = real (dRpsum(i))
174              pyd = aimag (dRpsum(i))
175              ssrd = (sx*sxd+sy*syd)/sr          ! |Rs|'
176              pprd = (px*pxd+py*pyd)/pr          ! |Rp|'
177              sdel = (sx*syd-sy*sxd)/(sr*sr)          ! delta(s)'
178              pdel = (px*pyd-py*pxd)/(pr*pr)          ! delta(p)'
179
180              ddel = pdel-sdel          ! delta'
181              dpsi = (sr*pprd-pr*ssrd)/(sr*sr+pr*pr)          ! psi'
182
183              a(k+1) = dpsi          ! d(psi ) /d(e)
184              a(k+2) = ddel          ! d(delta) /d(e)
185              k = k+2
186          end do
187
188          2 continue
189
190          sxd = real (dRsa)          ! incident angle
191          syd = aimag (dRsa)
192          pxd = real (dRpa)
193          pyd = aimag (dRpa)
194          ssrd = (sx*sxd+sy*syd)/sr          ! |Rs|'
195          pprd = (px*pxd+py*pyd)/pr          ! |Rp|'
196          sdel = (sx*syd-sy*sxd)/(sr*sr)          ! delta(s)'
197          pdel = (px*pyd-py*pxd)/(pr*pr)          ! delta(p)'
198
199          ddel = pdel-sdel          ! delta'
200          dpsi = (sr*pprd-pr*ssrd)/(sr*sr+pr*pr)          ! psi'
201
202          c(1) = dpsi          ! d(psi ) /d(angle),   Jacobian
203          c(2) = ddel          ! d(delta) /d(angle),   Jacobian
204 c      -----
205          sxd = real (dRsw)          ! frequency
206          syd = aimag (dRsw)
207          pxd = real (dRpw)
208          pyd = aimag (dRpw)
209          ssrd = (sx*sxd+sy*syd)/sr          ! |Rs|'

```



```

210      pprd = (px*pxd+py*pyd)/pr      ! |Rp|'
211      sdel = (sx*syd-sy*sxd)/(sr*sr) ! delta(s)'
212      pdel = (px*pyd-py*pxd)/(pr*pr) ! delta(p)'
213
214      ddel = pdel-sdel                ! delta'
215      dpsl = (sr*pprd-pr*ssrd)/(sr*sr+pr*pr) ! psi'
216
217      c(3) = dpsl                     ! d(psi )/dw
218      c(4) = ddel                     ! d(delta)/dw
219
220      return
221      end

```

6.2.16 SCATT0.FOR

```

1      subroutine scatt0 (wavlen, anglei, isampl, izsmpl, imbien, mvari)
2
3      include 'iounit.'
4      include 'defnit.'
5      include 'filmmm.'
6      include 'arrayd.'
7      include 'arrays.'
8      include 'filmss.'          ! z,e
9      include 'rstack.'          ! R, dR
10     include 'abcdef.'          ! a,b,c ----> output results
11     include 'handyy.'          ! pi,cccc,wavlev
12
13
14     imixtr = mixmbn(imbien)      ! mixture used as ambient
15     air = sqrt (real (dielec (imixtr))) ! refractive index, FILMSS
16
17     if (wavlen .lt. 0.0) then    ! wavelength, nm
18         qqg = -(pi+pi)/wavlen   !      inverse nm
19     else                        ! energy, eV
20         qqg = (pi+pi)*wavlen/wavlev !      inverse nm
21     end if
22
23     call forwr0 (qqg, anglei)    ! R only
24
25     sx = real (Rs)
26     sy = aimag (Rs)
27     px = real (Rp)
28     py = aimag (Rp)
29     call polar (sx,sy,sr,sa,1)
30     call polar (px,py,pr,pa,1)
31
32     if (sr.eq.0.0) then
33         if (pr.eq.0.0) then
34             psi = 0.0
35         else
36             psi = 0.5*pi
37         end if
38     else if (pr.eq.0.0) then    ! sr > 0.0
39         psi = 0.0
40     else if (pr.le.sr) then
41         psi = atan (pr/sr)
42     else
43         psi = 0.5*pi - atan(sr/pr)
44     end if
45
46     delta = pa-sa
47     1 if (delta.lt.0.0) then
48         delta = delta+2.0
49         goto 1
50     else if (delta.ge.2.0) then

```

```
51         delta = delta-2.0
52         goto 1
53     end if
54     delta = delta*pi
55
56     b(1) = psi           ! radians
57     b(2) = delta        ! radians
58
59     return
60 end
```

6.2.17 FORWRD.FOR

```

1      subroutine forwrd (qqq, angl)
2      real    qqq, angl
3
4      include 'defnit.'          ! nfilms, nrows
5      include 'filmss.'         ! z, e
6      include 'rstack.'         ! R, dR      ----> output results
7
8      complex ys(nfilms+1), eta(nfilms+1)
9      complex yp(nfilms+1), cta(nfilms+1)
10     complex ee(nfilms), em(nfilms), ep(nfilms), zq(nfilms)
11
12     complex half,one,two,four, eta0,eta0a, cta0,cta0a
13     complex top,bot,ss,pp, ssz,ppz,sse,ppe,ssa,ppa, pp1,pp2,pp3
14
15 c      Solve:   the direct or forward problem.
16 c      Discern: the reflection coefficient and Jacobian.
17 c      Given:   dielectric function of films (isotropic,homogeneous,uniform)
18 c              incident angle:   angl " radians
19 c              wavenumber:       qqq " 2*pi/wavelength
20 c              wavelength:       nano-meters
21
22 c      Find:    Rs, Rp.      ----> (psi, delta)
23 c              dRs,dRp.     <----- partial wrt:   (z, dielectric function)
24 c              dRsa,dRpa    <----- partial wrt:   -[n(air)*sin(angle)]**2
25 c              <----- partial wrt:   incident angle in radians
26 c              dRs,q,dRp,q  <----- partial wrt:   q " wavenumber
27
28     half = cmplx (0.5, 0.0)
29     one  = cmplx (1.0, 0.0)
30     two  = cmplx (2.0, 0.0)
31     four = cmplx (4.0, 0.0)
32
33     sa = sin (angl)
34     ca = cos (angl)
35     as = air*sa
36     ac = air*ca
37     as2 = as*as                      ! air
38
39     eta0 = cmplx ( ac, 0.0)          ! air   TE
40     eta0a = cmplx (-as, 0.0)        ! air   d(eta)/d(angl)
41     cta0 = cmplx ( ca/air, 0.0)     ! air   TM
42     cta0a = cmplx (-sa/air, 0.0)    ! air   d(cta)/d(angl)
43
44     mfilms = mfilm+1                ! films, substrate
45
46     do i=1,mfilms                   ! films, substrate
47         eta(i) = sqrtt (die(i)-cmplx(as2,0.0)) ! TE
48         cta(i) = eta(i)/die(i)        ! TM
49     end do
50

```

```

51 c      Determine the reflection coefficients in air.
52 c      Method for TE:  admittance = Y = - Hx/Ey,      Rs uses E field.
53 c      TM:      impedance = Z =   Ex/Hy,      Rp uses H field.
54
55      ys(mfilms) = eta(mfilms)      ! substrate
56      yp(mfilms) = cta(mfilms)
57      if (mfilm.ne.0) then
58          do i=mfilm,1,-1      ! backwards
59              x = zzz(i)*qqq
60              zq(i) = cmplx (0.0, x)      ! izq
61              ss = cmplx (0.0, x+x) * eta(i)      ! izqn2
62              x = exp (real (ss))
63              y = aimag (ss)
64              ss = cmplx (x*cos(y), x*sin(y))      ! exp (izqn2)
65              ee(i) = ss
66              em(i) = one-ss
67              ep(i) = one+ss
68              ys(i) = eta(i)* ((em(i)*eta(i)+ep(i)*ys(i+1)) /
69              &                  (ep(i)*eta(i)+em(i)*ys(i+1)) )
70              yp(i) = cta(i)* ((em(i)*cta(i)+ep(i)*yp(i+1)) /
71              &                  (ep(i)*cta(i)+em(i)*yp(i+1)) )
72          end do
73      end if
74      Rs = (eta0-ys(1)) /(eta0+ys(1))      ! air
75      Rp = (cta0-yp(1)) /(cta0+yp(1))      ! air
76
77 c      Jacobian
78
79      dRs = cmplx (0.0,0.0)      ! d/dq
80      dRp = cmplx (0.0,0.0)
81
82      do i=mfilms,1,-1      ! backwards
83          if (i.eq.mfilms) then      ! source substrate
84              sse = half /eta(i)      ! d(eta)/d(e)
85              ssa = sse      ! d(eta)/d(-as**2)
86              ssz = cmplx (0.0,0.0)      ! convenience
87
88              ppe = (cmplx (2.0*as2, 0.0) - die(i))
89              &      * half / (eta(i)* die(i)*die(i))      ! d(cta)/d(e)
90              ppa = half / (eta(i)*die(i))      ! d(cta)/d(-as**2)
91              ppz = cmplx (0.0,0.0)      ! convenience
92          else      ! source film
93              bot = ep(i)*eta(i) + em(i)*ys(i+1)      ! denominator, TE
94              top = em(i)*eta(i) + ep(i)*ys(i+1)      ! numerator
95              ss = em(i) + zq(i)*ee(i)*(ys(i+1)-eta(i))
96              &      + ep(i)*half*(ys(i+1)/eta(i))
97              pp = ep(i)*half - zq(i)*ee(i)*(ys(i+1)-eta(i))
98
99              sse = (ss/bot) - (pp*top)/(bot*bot)
100             ssa = (ss + ep(i)*eta(i)*ssa) /bot -
101             &      (pp + em(i)*eta(i)*ssa)*top /(bot*bot)
102             ssz = two*ee(i)* (ys(i+1)-eta(i)) * (ys(i+1)+eta(i))
103             &      * (eta(i)/bot)**2      ! d/d (izq2)

```



```

104
105      bot = ep(i)*eta(i) + em(i)*yp(i+1)*die(i)      ! denominator, TM
106      top = em(i)*eta(i) + ep(i)*yp(i+1)*die(i)      ! numerator
107      pp = (cmplx (2.0*as2, 0.0) - die(i))
108      &      * half / (eta(i)* die(i)*die(i))          ! d(cta)/d(e)
109
110      pp1 = pp*top/bot
111      pp2 = em(i)*half/die(i) + ep(i)*cta(i)*yp(i+1) +
112      &      zq(i)*ee(i)*(yp(i+1)-cta(i))
113      pp3 = ep(i)*half/die(i) + em(i)*cta(i)*yp(i+1) -
114      &      zq(i)*ee(i)*(yp(i+1)-cta(i))
115      ppe = pp1 + pp2/bot - pp3*top/(bot*bot)
116
117      pp1 = half*top / (bot*eta(i)*die(i))
118      pp2 = em(i)*half/die(i) + ep(i)*eta(i)*ppa + ,
119      &      zq(i)*ee(i)*(yp(i+1)-cta(i))
120      pp3 = ep(i)*half/die(i) + em(i)*eta(i)*ppa -
121      &      zq(i)*ee(i)*(yp(i+1)-cta(i))
122      ppa = pp1 + pp2/bot - pp3*top/(bot*bot)
123
124      pp = (eta(i)-die(i)*yp(i+1)) * (eta(i)+die(i)*yp(i+1))
125      ppz = -two*ee(i)*eta(i)*cta(i)* (pp/(bot*bot))
126      end if
127
128      if (i.ne.1) then                                ! transport
129          k = i-1
130          do j=k,1,-1                                ! backwards
131              ss = eta(j) / (ep(j)*eta(j)+em(j)*ys(j+1))
132              pp = cta(j) / (ep(j)*cta(j)+em(j)*yp(j+1))
133              ss = four*ee(j)*ss*ss                    ! coefficient
134              pp = four*ee(j)*pp*pp
135              sse = sse*ss                              ! Y'(e)
136              ppe = ppe*pp
137              ssz = ssz*ss                              ! Y'(izq2)
138              ppz = ppz*pp
139          end do
140      end if
141      ss = -two*eta0 / ((eta0+ys(1))**2)                ! coefficient
142      pp = -two*cta0 / ((cta0+yp(1))**2)
143      sse = sse*ss                                      ! R'(e)
144      ppe = ppe*pp
145      ssz = ssz*ss                                      ! R'(izq2)
146      ppz = ppz*pp
147
148      c      The format of the Jacobian vector has the form:
149      c      air / film#1 / film#2 / ... / mfilm / substrate
150      c      [z,e,      z,e,      ...  z,e,      e]
151
152      k = 2*(i-1)                                       ! position Jacobian
153      if (i.eq.mfilms) then                             ! substrate, ( ,e)
154          k = k-1
155      else                                             ! film,      (z,e)
156          ss = cmplx (0.0, qq*2.0)                    ! d(izq2) / dz

```

```

157      dRs(k+1) = ssz*ss      ! R'(z)
158      dRp(k+1) = ppz*ss      ! R'(z)
159
160      ss = cmplx (0.0, zzz(i)*2.0)      ! d(izq2) /dq
161      dRsq = dRsq+ssz*ss      ! R'(q)
162      dRpq = dRpq+ppz*ss      ! R'(q)
163      end if
164      dRs(k+2) = sse      ! R'(e)
165      dRp(k+2) = ppe      ! R'(e)
166
167      end do      ! mfilms
168
169
170 c      Since the angular partials involved:      dR/d (-(air*sin)**2)
171 c      and we want partials wrt angle, i.e.:      dR/d (angl)      angl`radians
172
173      ss = cmplx (-as*ac*2.0, 0.0)      ! d (-(air*sin)**2) /d(angl)
174      ssa = ssa*ss      ! d(Ys) /d(angl)
175      ppa = ppa*ss      ! d(Yp) /d(angl)
176
177      ssa = two* (eta0a*ys(1)-eta0*ssa) /((eta0+ys(1))**2)      ! R'(a)
178      ppa = two* (cta0a*yp(1)-cta0*ppa) /((cta0+yp(1))**2)
179      dRsa = ssa      ! R'(a)
180      dRpa = ppa
181
182 c      Note one distinction regarding conventions in defintions of fields.
183 c      The TM calculation utilizes H fields, Rp = H( reflected)/H( incident),
184 c      while some conventions use E fields, Rp = E(x,reflected)/E(x,incident).
185 c      Consequently, in order to change to this other convention, one should
186 c      induce a minus sign (-) onto the terms of Rp.
187
188 c*      k = 2*mfilm+1
189 c*      do i=1,k
190 c*          dRp(i) = -dRp(i)
191 c*      end do
192 c*      dRpa = -dRpa
193 c*      dRpq = -dRpq
194 c*      Rp = -Rp
195
196      return
197      end

```

6.2.18 FORWR0.FOR

```

1      subroutine forwr0 (qqq, angl)
2      real                      qqq, angl
3
4      include  'defnit.'          ! nfilms, nrows
5      include  'filmss.'          ! z, e
6      include  'rstack.'          ! R, dR      -----> output results
7
8      complex  ys(nfilms+1), eta(nfilms+1)
9      complex  yp(nfilms+1), cta(nfilms+1)
10     complex  ee(nfilms), em(nfilms), ep(nfilms), zq(nfilms)
11
12     complex  half, one,  eta0, cta0
13     complex  top, bot, ss, pp,  ssz, ppz, sse, ppe, ssa, ppa,  pp1, pp2, pp3
14
15 c      Solve:    the direct or forward problem.
16 c      Discern:  the reflection coefficient and Jacobian.
17 c      Given:    dielectric function of films (isotropic, homogeneous, uniform)
18 c                incident angle:    angl  " radians
19 c                wavenumber:        qqq  " 2*pi/wavelength
20 c                wavelength:        nano-meters
21
22 c      Find:      Rs, Rp.      -----> (psi, delta)
23 c                dRs, dRp.    <----- partial wrt:  (z, dielectric function)
24 c                dRsa, dRpa    <----- partial wrt:  -[n(air)*sin(angle)]**2
25 c                <----- partial wrt:  incident angle in radians
26 c                dRsq, dRpq    <----- partial wrt:  q  " wavenumber
27
28     half = cmplx (0.5, 0.0)
29     one  = cmplx (1.0, 0.0)
30
31     sa = sin (angl)
32     ca = cos (angl)
33     as = air*sa
34     ac = air*ca
35     as2 = as*as                      ! air
36
37     eta0 = cmplx ( ac, 0.0)          ! air  TE
38     cta0 = cmplx ( ca/air, 0.0)      ! air  TM
39
40     mfilms = mfilm+1                ! films, substrate
41
42     do i=1,mfilms                   ! films, substrate
43         eta(i) = sqrtt (die(i)-cmplx(as2,0.0)) ! TE
44         cta(i) = eta(i)/die(i)        ! TM
45     end do
46
47 c      Determine the reflection coefficients in air.
48 c      Method for TE:  admittance = Y = - Hx/Ey,      Rs uses E field.
49 c                      TM:  impedance = Z =  Ex/Hy,    Rp uses H field.
50

```

```

51     ys(mfilms) = eta(mfilms)           ! substrate
52     yp(mfilms) = cta(mfilms)
53     if (mfilm.ne.0) then
54         do i=mfilm,1,-1                 ! backwards
55             x = zzz(i)*qqq
56             zq(i) = cmplx (0.0, x)       ! izq
57             ss = cmplx (0.0, x+x) * eta(i) ! izqn2
58             x = exp (real (ss))
59             y = aimag (ss)
60             ss = cmplx (x*cos(y), x*sin(y)) ! exp (izqn2)
61             ee(i) = ss
62             em(i) = one-ss
63             ep(i) = one+ss
64             ys(i) = eta(i)* ((em(i)*eta(i)+ep(i)*ys(i+1)) /
65 &                             (ep(i)*eta(i)+em(i)*ys(i+1)) )
66             yp(i) = cta(i)* ((em(i)*cta(i)+ep(i)*yp(i+1)) /
67 &                             (ep(i)*cta(i)+em(i)*yp(i+1)) )
68         end do
69     end if
70     Rs = (eta0-ys(1)) /(eta0+ys(1))      ! air
71     Rp = (cta0-yp(1)) /(cta0+yp(1))      ! air
72
73     return
74     end

```

6.2.19 DIFFER.FOR

```

1      subroutine differ (exprmt, theory, diff)                ! radians
2      real  exprmt, theory, diff
3      include 'handyy.'                ! pi
4
5
6      x1 = exprmt - theory                ! 0 .le. theory .lt. 2*pi
7      x2 = x1 - (pi+pi)                ! mod 2*pi
8      x3 = x1 + (pi+pi)
9
10     a1 = abs (x1)
11     a2 = abs (x2)
12     a3 = abs (x3)
13
14     if (a1.le.a2) then                ! a1 < a2
15         diff = x1
16         if (a3.lt.a1) then
17             diff = x3
18         end if
19     else                ! a2 < a1
20         diff = x2
21         if (a3.lt.a2) then
22             diff = x3
23         end if
24     end if
25
26     return
27     end

```


6.2.20 STAT22.FOR

```

1      subroutine stat22 (n,b)
2      real      b(n)
3      include  'iounit.'
4      include  'handyy.'          ! pi
5      logical   llzero
6
7  c      Perform:    simple statistics of deviations from the model.
8  c      Discern:    (mean, standard deviation)      of deviations.
9  c      Assume:     b(1) = d(psi ) = deviation = experiment-model
10 c                b(2) = d(delta) = deviation = experiment-model
11
12      raddeg = 180.0 / pi          ! degrees <--- radians
13      nh = n/2                    ! psi, delta
14      h = float (nh)
15
16      write (iout,111)
17      if (n.le.1 .or. n.ge.nh+nh) then
18          write (iout,112) n
19          stop
20      end if
21
22      a1 = 0.0
23      a2 = 0.0
24      do i=1,n,2                  ! mean deviation
25          a1 = a1 + b(i )         !     psi
26          a2 = a2 + b(i+1)        !     delta
27      end do
28      a1 = a1 /h                  !     psi
29      a2 = a2 /h                  !     delta
30
31      llzero = .false.           ! zero variance
32      s1 = 0.0
33      s2 = 0.0
34      s3 = 0.0
35      do i=1,n,2                  ! variance of deviations
36          s1 = s1 + (b(i )-a1)**2  !     psi
37          s2 = s2 + (b(i+1)-a2)**2 !     delta
38          s3 = s3 + (b(i+1)-a2)*(b(i)-a1) !     correlation
39      end do
40      s1 = sqrt (s1 /h)           ! standard deviation
41      s2 = sqrt (s2 /h)
42      s3 =      s3 /h            ! covariance
43
44      if (s1.eq.0.0 .or. s2.eq.0.0) then ! exact fit, no scatter
45          llzero = .true.
46      else
47          s3 = s3 /(s1*s2)        ! correlation coefficient
48      end if
49
50      a1 = a1 *raddeg            ! degrees

```

```

51      a2 = a2 *raddeg
52      s1 = s1 *raddeg
53      s2 = s2 *raddeg
54
55      write (iout,113) a1,s1, a2,s2, s3
56      if (llzero) write (iout,114)
57
58      return
59
60      111 format (/ 1x, 15('----'))
61      &      /' Statistics of deviations " experiment-model " g'
62      &      /'      where:  g is a column vector of length 2M,'
63      &      /'      () denotes either (delta) or (psi)'
64      &      /'      mean () = m() = <g()> = (1/M) sum: g()'
65      &      /'      variance () = < (g() -m() )**2 >      '
66      &      /'      covariance = < (g(1)-m(1))*(g(2)-m(2)) >      '
67      &      /'      std dev = sqrt (variance)      '
68      &      /'      correlat coef = covariance / (sd(1) * sd(2))      ' )
69
70      112 format (/ stat22, ... oops " inconsistency, n=', i5)
71
72      113 format (/ 20x, ' mean,', 4x, ' std dev      (degrees)'
73      &      / 5x, ' psi:', 4x, f10.3, 3x, f10.3
74      &      / 5x, 'delta:', 4x, f10.3, 3x, f10.3
75      &      / 5x, 6x, 4x, f10.3, 1x,
76      &      ' " correlation coefficient " <psi|delta>      ')
77      114 format ( 26x, ' " UNnormalized, because atleast one of the '
78      &      / 26x, '      standard deviations vanish.'/)
79
80      end

```

6.2.21 CORLAT.FOR

```

1      subroutine corlat
2
3      c      Construct the correlation matrix for model parameters (z,f,p)
4      c      for the given sampling of measurementd data from experiment.
5      c      Correlation matrix " normalized:  [J(Transpose)*J].
6
7      include 'iounit.'
8      include 'defnit.'
9      include 'filmmm.'
10     include 'arrays.'          ! aa
11     include 'wstack.'          ! aat
12     include 'handyy.'          ! pi
13
14     real      det(2)            ! LINPACK
15     integer   inert(3)          ! LINPACK
16
17
18     llnorm = .false.            ! UNscaled by experiment
19     call asmb1                  ! ia,ja,aa,bb
20     call stat22 (meqns,bb)      ! mean, std dev
21     call norm  (meqns,bb,bbnorm,0) ! |<gg>|
22     bbnorm = bbnorm/sqrt (float (meqns-mvary)) ! variance, <gg>/(2M-N)
23     raddeg = 180.0/pi          ! degree/radian
24
25     kv = 0
26     do jv=1,mvary              ! A(T)*A,      parameters
27         do iv=1,jv              ! upper triangle + diagonal
28             sum = 0.0
29             do i=1,meqns,2
30                 j1 = ia(i )
31                 j2 = ia(i+1)-1
32                 mv = j2-j1+1
33                 s1 = 0.0
34                 s2 = 0.0
35                 s3 = 0.0
36                 s4 = 0.0
37                 do j=j1,j2      ! within a row of A
38                     jaj = ja(j) ! column
39                     if (jaj.eq.iv) then
40                         s1 = aa(j )
41                         s3 = aa(j+mv)
42                     end if
43                     if (jaj.eq.jv) then
44                         s2 = aa(j )
45                         s4 = aa(j+mv)
46                     end if
47                 end do
48                 sum = sum + s1*s2 + s3*s4 ! dot product
49             end do
50             sum = sum/float (meqns)      ! convenience

```

```

51         kv = kv+1                                ! packed format - storage
52         aat(kv) = sum                             ! upper triangle + diagonal
53         if (jv.eq.iv) then                         ! diagonal
54             xx(jv) = sqrt(sum)
55         end if
56     end do
57 end do
58
59 kv = 0
60 do jv=1,mvary                                     ! correlation matrix
61     do iv=1,jv                                     ! renormalize
62         kv = kv+1
63         aat(kv) = aat(kv)/(xx(jv)*xx(iv))
64     end do
65 end do
66
67 write (iout,211)
68 k2 = 0
69 do i=1,mvary
70     k1 = k2+1
71     k2 = k2+i
72     write (iout,212) i, (aat(k), k=k1,k2)
73 end do
74 write (iout,214)
75 write (iout,215) (xx(i), i=1,mvary)              ! scaling coefficients
76
77 c -----
78 c LINPACK, Chapter 5, Solving symmetric indefinite matrices.
79
80 call sspco (aat, mvary, ipvt, rcond, w)           ! UD*T(U) decomposition
81 write (iout,216) rcond                           ! inverse condition number
82
83 c* if (1.0 .eq. 1.0+rcond ) then                  ! singular matrix
84 if (1.0 .ne. 1.0+rcond*0.01) then                 ! NOT ill-conditioned
85     call sspdi (aat, mvary, ipvt, det, inert, w, 111)
86     write (iout,217) det, inert
87     k2 = 0
88     do i=1,mvary
89         k1 = k2+1
90         k2 = k2+i
91         write (iout,213) i, (aat(k), k=k1,k2)
92     end do
93 else                                              ! indeterminate
94     return                                         ! no reason to continue
95 end if
96
97 c -----
98 c Estimate the uncertainty in the model parameters.
99 c Ignore correlation among model parameters,
100 c i.e., consider only the diagonal contributions.
101
102 k2 = 0
103 do i=1,mvary

```

```

104         k1 = k2+1
105         k2 = k2+i                                ! diagonal
106         xx(i) = bbnorm*sqrt (aat(k2)) /xx(i)
107     end do
108     bbnorm = bbnorm*raddeg                          ! degrees
109
110     write (iout,121) bbnorm
111     do i=1,mvary
112         j = iptu(i)
113         if (j .le. mfilmz) then                      ! widths
114             write (iout,122) i, widths(j), xx(i), j
115         else if (j .le. mfilmz+mlmnts) then          ! fractions
116             j = j-mfilmz
117             write (iout,123) i, fflmnt(j), xx(i), j
118         else                                          ! parameters
119             j = j-mfilmz-mlmnts
120             write (iout,124) i, rrparm(j), xx(i), j
121         end if
122     end do
123
124     return
125
126 121 format (/ 1x, 15('----'))
127 &          /' The standard deviation of the residuals.'
128 &          //' s(g) = sqrt [<gg>/((2M-N)] =', 1p1e14.5,' (degrees)'
129 &          //' The estimated uncertainty in the model parameters, '
130 &          /' assuming no correlation, i.e., diagonal terms only.'
131 &          // 17x, 'value,'          3x, 'uncertainty.' )
132 122 format (1x, i5, ' '), f15.4, f15.5, ' ', for:', i5, ' " (z,zu)')
133 123 format (1x, i5, ' '), f15.4, f15.5, ' ', for:', i5, ' " (f,fu)')
134 124 format (1x, i5, ' '), f15.4, f15.5, ' ', for:', i5, ' " (p,pu)')
135
136 211 format (/ ' [J(T)*J], renormalized for correlation.')
137 212 format (1x, i4, ' '), 1x, 10f10.5, : /(7x, 10f10.5))
138 213 format (1x, i4, ' '), 1x, 1p10e10.2, : /(7x, 10e10.2))
139 214 format (/ ' Normalization coefficients, sqrt: [J(T)*J]_(i,i)')
140 215 format ( 1x, 1p10e10.2)
141
142 216 format (/ ' rcond = ', 1p1e10.2, ' ', condition number, [J(T)*J]')
143 217 format (/ ' [J(T)*J]**(-1): '
144 &          /' Determinant: ', f8.4, ' E ', f8.4
145 &          /' Inertia: (' , 3i4, ' ), '
146 &          ' number of (+,-,0) eigenvalues.'
147 &          /' Inverse: upper+diagonal matrix')
148
149     end

```


6.3 General Utilities

6.3.1 DOT.FOR

```
1      subroutine dot (n,x,y, xy,k)
2      real          x(1), y(1)
3
4      xy = 0.0
5      xn = 0.0
6      yn = 0.0
7      do i=1,n          ! find maximum
8          xn = amax1 (xn, abs (x(i)))
9          yn = amax1 (yn, abs (y(i)))
10     end do
11     if (xn.eq.0.0 .or. yn.eq.0.0) return
12
13     xs = 0.0
14     ys = 0.0
15     do i=1,n
16         xx = x(i)/xn      ! scaled vector component
17         yy = y(i)/yn
18         xs = xs + xx*xx    ! dot product " |x*x|
19         ys = ys + yy*yy    ! dot product " |y*y|
20         xy = xy + xx*yy    ! dot product " |x*y|
21     end do
22
23     h = float (n)
24     xs = xs/h              ! mean square value
25     ys = ys/h
26     xy = xy/h
27     xs = sqrt (xs)         ! root mean square value
28     ys = sqrt (ys)
29
30     if (k.eq.0) then       ! usual dot product
31         xy = xy*xn*yn*h
32     else if (k.eq.1) then  ! un-normalized
33         xy = xy*xn*yn
34     else                   ! normalized
35         xy = xy/(xs*ys)
36     end if
37
38     return
39     end
```

6.3.2 NORM.FOR

```
1      subroutine norm (n,x, xn,k)
2      real x(1)
3
4      xn = 0.0
5      do i=1,n                      ! find maximum
6          xn = amax1 (xn, abs (x(i)))
7      end do
8      if (xn .eq. 0.0) return
9
10     xx = 0.0
11     do i=1,n                      ! dot product
12         xx = xx + (x(i)/xn)**2      ! |x*x|
13     end do
14
15     if (k.eq.1) then              ! mean squared value
16         xx = xx/float (n)
17     end if
18     xn = xn*sqrt (xx)              ! Euclidean norm
19
20     return
21     end
```

6.3.3 APROD.FOR

```

1      subroutine aprod (mode,m,n,x,y, ia,ja,aa)
2      integer    mode, m, n, ia(1), ja(1)
3      real       x(n), y(m), aa(1)
4      data       iout / 6 /
5
6      c -----
7      c      A = A(m,n),      Transpose operator = (')
8      c      Operation:      mode= 1,      set:  y = y + A *x
9      c                      mode= 2,      set:  x = x + A'*y
10     c                      x' = x' + y'*A
11     c -----
12
13     if (mode.eq.1) then                ! y = y + Ax
14         do i=1,m                      ! scan rows of matrix A
15             mj = ia(i+1)-ia(i)        ! number of columns in row
16             if (mj.ne.0) then
17                 ss = 0.0                ! sum
18                 jj = ia(i)-1           ! indexing
19                 do j=1,mj              ! scan columns of row
20                     jj = jj+1
21                     kk = ja(jj)        ! column
22                     ss = ss + aa(jj)*x(kk)
23                 end do
24                 y(i) = y(i)+ss         ! y = y+Ax
25             end if
26         end do
27
28     else if (mode.eq.2) then            ! x' = x' + y'*A
29         do i=1,m                      ! scan rows of matrix A
30             mj = ia(i+1)-ia(i)        ! number of columns in row
31             if (mj.ne.0) then
32                 yy = y(i)
33                 jj = ia(i)-1           ! indexing
34                 do j=1,mj              ! scan columns of row
35                     jj = jj+1
36                     kk = ja(jj)        ! column
37                     x(kk) = x(kk) + yy*aa(jj)
38                 end do
39             end if
40         end do
41
42     else
43         write (iout,10) mode
44         stop
45     end if
46
47     return
48
49 10 format (/ ' aprod, ... error, mode= ', i2)
50     end

```

6.3.4 SCALII.FOR

```

1      subroutine scalii (m,n, ia,ja,a,b, p,k)
2      integer    ia(1), ja(1), m, n, k
3      real       a(1), b(1), p(1)
4
5      c  -----
6      c  Scale the rows in matrix,      A(m,n), b(m).
7      c  Retain scaling coefficients in P(m).
8      c  Evaluate P only when k = 0,1,2,3.
9      c  Re-scale A only when |k| = 2,3.
10     c  Re-scale B only when |k| = 1, 3.
11     c  Matrix A is stored (row-wise) in the Yale Sparse Matrix Format.
12     c  -----
13
14     ka = iabs (k)
15     if (ka.gt.3) then
16         do i=1,m
17             p(i) = 1.0
18         end do
19         return
20     end if
21
22     if (k.ge.0) then
23         do i=1,m
24             mj = ia(i+1)-ia(i)
25             if (mj.ne.0) then
26                 big = 0.0
27                 jj = ia(i)-1
28                 do j=1,mj
29                     jj = jj+1
30                     big = amax1 (big, abs (a(jj)))
31                 end do
32                 if (big .eq. 0.0) then
33                     p(i) = 1.0
34                 else
35                     ss = 0.0
36                     jj = jj-mj
37                     do j=1,mj
38                         jj = jj+1
39                         ss = ss + (a(jj)/big)**2
40                     end do
41                     p(i) = big*sqrt (ss)
42                 end if
43             end if
44         end do
45     end if
46
47     if (ka.eq.2 .or. ka.eq.3) then
48         do i=1,m
49             mj = ia(i+1)-ia(i)
50             if (mj.ne.0) then

```

```

51         pp = p(i)                                ! scale factor of row
52         jj = ia(i)-1                              ! indexing
53         do j=1,mj                                  ! scan columns in row
54             jj = jj+1
55             a(jj) = a(jj)/pp                        ! rescale the row
56         end do
57     end if
58 end do
59 end if
60
61 if (ka.eq.1 .or. ka.eq.3) then                    ! rescale b
62     do i=1,m                                       ! scan rows
63         b(i) = b(i)/p(i)
64     end do
65 end if
66
67 return
68 end

```


6.3.5 SCALJJ.FOR

```

1      subroutine scaljj (m,n, ia,ja,a,b, p,w,k)
2      integer      ia(1), ja(1), k, m, n
3      real         a(1), b(1), p(1), w(1)
4
5      c      -----
6      c      Scale matrix A so the diagonal of:      [Transpose(A)*A] = 1.
7      c      Matrix A is stored row-wise in the Yale Sparse Matrix Format.
8      c      Scale the columns of matrices, A(m,n), b(n).
9      c      Retain the scaling coefficients in      P(n).
10     c      Use as a dummy work storage array,      W(n).
11     c      Evaluate P only when      k = 0,1,2,3.
12     c      Re-scale A only when      |k| =      2,3.
13     c      Re-scale B only when      |k| =      1, 3.
14     c      -----
15
16     ka = iabs (k)                                ! convenience
17     if (ka.gt.3) then                             ! out of range
18         do j=1,n                                  ! scan columns
19             p(j) = 1.0                            !      default
20         end do
21         return
22     end if
23
24     if (k.ge.0) then                               ! determine scaling
25         do j=1,n                                  ! scan columns
26             p(j) = 0.0                            ! initialize
27             w(j) = 0.0                            ! sums
28         end do
29
30         do i=1,m                                  ! scan rows, A
31             mj = ia(i+1)-ia(i)                    ! number of columns in row
32             if (mj.ne.0) then
33                 jj = ia(i)-1                      ! indexing
34                 do j=1,mj                          ! scan columns of row
35                     jj = jj+1
36                     kk = ja(jj)                    ! column
37                     p(kk) = amax1 (p(kk), abs (a(jj))) ! max |A(:,j)|
38                 end do
39             end if
40         end do
41
42         do i=1,m                                  ! scan rows, A
43             mj = ia(i+1)-ia(i)                    ! number of columns
44             if (mj.ne.0) then
45                 jj = ia(i)-1                      ! indexing
46                 do j=1,mj                          ! scan columns in row
47                     jj = jj+1
48                     kk = ja(jj)                    ! column
49                     w(kk) = w(kk) + (a(jj)/p(kk))**2 ! sums
50                 end do

```

```

51         end if
52     end do
53
54     do j=1,n                                ! scan columns
55         p(j) = p(j)*sqrt (w(j))            ! retain scale factor
56     end do
57 end if
58
59 if (ka.eq.2 .or. ka.eq.3) then              ! rescale A
60     do i=1,m                                ! scan rows, A
61         mj = ia(i+1)-ia(i)                  ! number of columns
62         if (mj.ne.0) then
63             jj = ia(i)-1                    ! indexing
64             do j=1,mj                        ! scan columns in row
65                 jj = jj+1
66                 kk = ja(jj)                  ! column
67                 a(jj) = a(jj)/p(kk)          ! rescale column
68             end do
69         end if
70     end do
71 end if
72
73 if (ka.eq.1 .or. ka.eq.3) then              ! rescale b
74     do j=1,n                                ! scan columns
75         b(j) = b(j)/p(j)                    ! rescale column
76     end do
77 end if
78
79 return
80 end

```

6.3.6 CGNL.FOR

```

1      subroutine cgnl (ma,na,ia,ja,aa, b,x,
2      &                itmax, u,v,w, xx,se)
3
4      integer    ia(1), ja(1)
5      real       aa(1), b(1), x(1)
6      real       u(1), v(1), w(1), xx(1), se(1)
7      external   aprod
8      data       iout /6/
9
10     c  -----
11     c  real       b(ma), u(ma),          aa(ma,na)
12     c  real       x(na), v(na), w(na), xx(na), se(na)
13
14     c  Solve the linear or matrix algebra problem, Ax=b.
15     c  Matrix A is stored row-wise in the Yale Sparse Matrix Format.
16     c  Reference:   C.C.Paige and M.A.Saunders,
17     c  "LSQR:      An Algorithm for Sparse Linear Equations
18     c  and Sparse Least Squares",
19     c  Association for Computing Machinery,
20     c  Transactions on Mathematical Software,
21     c  Volume 8, Number 1, March 1982, pp. 43-71, (Note pp. 50-51).
22     c  ibid.,      Volume 8, Number 2, June 1982, pp. 195-209.
23     c  -----
24
25     loop = 0                                ! initialize
26     1 loop = loop+1                          ! update counter
27     rr = 0.0                                ! norm of residual
28     do i=1,ma                                ! scan rows, r=b-Ax
29         mj = ia(i+1)-ia(i)                  ! number of columns in row
30         if (mj .ne. 0) then
31             ss = 0.0                        ! initialize sum
32             jj = ia(i)-1                    ! indexing
33             do j=1,mj                        ! scan columns of row
34                 jj = jj+1
35                 kk = ja(jj)                 ! column
36                 ss = ss + aa(jj)*x(kk)      ! Ax
37             end do
38             ss = b(i)-ss                     ! r = b-Ax = residual
39             u(i) = ss                        ! r = residual
40             rr = rr+ss*ss                    ! |r|**2
41         end if
42     end do
43     if (rr .eq. 0.0) return
44
45     if (loop .eq. 1) then                    ! retain first norm
46         rrr = rr
47     else if (rr .ge. rrrlast*0.98) then      ! rate of convergence
48         ratio = sqrt (rr/rrr)
49         c* write (iout,103) loop, ratio
50         c* write (iout,104) istop, anorm, acond, rnorm, arnorm, xnorm

```

```

51      return
52  end if
53  rrlast = rr                                ! update
54
55  c----- ! Set-up for LSQR
56  relpr = 1.0E-06 ! relative precision of floating point arithmetic
57  damp = 1.0E+00 !
58  atol = 1.0E-06 ! relative error of data in A
59  btol = 1.0E-06 ! relative error of data in B ~ rhs
60  conlim = 1.0E+04 ! apparent condition number of matrix A-bar
61                  ! (upper limit)
62  itnlim = itmax ! upper limit on number of iterations
63  nout = -iout ! output index to printer
64
65  call lsqr (ma, na, aprod, damp,
66  &          ia, ja, aa,
67  &          u, v, w, xx, se,
68  &          atol, btol, conlim, itnlim, nout,
69  &          istop, anorm, acond, rnorm, arnorm, xnorm)
70
71  do i=1,na
72      x(i) = x(i) + xx(i) ! update solution
73      xx(i) = 0.0 ! reset
74  end do
75  goto 1 ! loop back
76
77  101 format (' cgnl, singular row= ', i10)
78  102 format (' cgnl, singular column= ', i10)
79  103 format (' cgnl, ', i5, 1p1e11.3, ' ~ loop, ratio '
80  &          , '(residual reduction)')
81  104 format (' cgnl, ', i5, 1p5e11.3)
82  end

```

6.3.7 LSQR.FOR

The following subroutine is located in the software library,

Guide to Available Mathematical Software, by R. F. Boisvert, S. E. Howe, and D. K. Ka-
haner, Center for Applied Mathematics, National Institute of Standards and Tech-
nology (formerly National Bureau of Standards), U.S. Department of Commerce,
1985.

The source code is copyrighted by the Association for Computing Machinery, Inc. The
references for the following source code include:

- 1) C. C. Paige and M. A. Saunders, "LSQR: An Algorithm for Sparse Linear Equations
and Sparse Least Squares," *ACM Trans. Math. Softw.* 8, 43-71 (1982).
- 2) C. C. Paige and M. A. Saunders, "Algorithm 583, LSQR: Sparse Linear Equations
and Least Squares Problems," *ACM Trans. Math. Softw.* 8, 195-209 (1982).

```
1      SUBROUTINE LSQR (M,N,APROD,DAMP,
2      1      IA,JA,AA,
3      2      U,V,W,X,SE,
4      3      ATOL,BTOL,CONLIM,ITNLIM,NOUT,
5      4      ISTOP,ANORM,ACOND,RNORM,ARNORM,XNORM )
6  C
7      EXTERNAL  APROD
8      INTEGER   M,N,ITNLIM,NOUT,ISTOP
9      INTEGER   IA(M),JA(M)
10     REAL      AA(M),                U(M),V(N),W(N),X(N),SE(N),
11     1      ATOL,BTOL,CONLIM,DAMP,ANORM,ACOND,RNORM,ARNORM,XNORM
12  C -----
13  C
14  C      LSQR  FINDS A SOLUTION  X  TO THE FOLLOWING PROBLEMS...
15  C
16  C      1. UNSYMMETRIC EQUATIONS --      SOLVE  A*X = B
17  C
18  C      2. LINEAR LEAST SQUARES  --      SOLVE  A*X = B
19  C                                          IN THE LEAST-SQUARES SENSE
20  C
21  C      3. DAMPED LEAST SQUARES  --      SOLVE  (  A  ) * X = ( B )
22  C                                          ( DAMP*I )   ( 0 )
23  C                                          IN THE LEAST-SQUARES SENSE
24  C
25  C      WHERE  A  IS A MATRIX WITH  M  ROWS AND  N  COLUMNS,
26  C      B  IS AN M-VECTOR, AND
27  C      DAMP  IS A SCALAR (ALL QUANTITIES REAL).
28  C      THE MATRIX  A  IS INTENDED TO BE LARGE AND SPARSE.
29  C      IT IS ACCESSED BY MEANS OF SUBROUTINE CALLS OF THE FORM
```



```

30 C
31 C      CALL APROD ( MODE,M,N,X,Y,  IA,JA,AA )
32 C
33 C      WHICH MUST PERFORM THE FOLLOWING FUNCTIONS...
34 C
35 C          IF MODE = 1, COMPUTE  Y = Y + A*X.
36 C          IF MODE = 2, COMPUTE  X = X + A(TRANPOSE)*Y.
37 C
38 C      THE VECTORS X AND Y ARE INPUT PARAMETERS IN BOTH CASES.
39 C      IF MODE = 1, Y SHOULD BE ALTERED WITHOUT CHANGING X.
40 C      IF MODE = 2, X SHOULD BE ALTERED WITHOUT CHANGING Y.
41 C      THE PARAMETERS:  IA, JA, AA.
42 C      MAY BE USED FOR WORKSPACE AS DESCRIBED BELOW.
43 C
44 C      THE RHS VECTOR B IS INPUT VIA U, AND SUBSEQUENTLY OVERWRITTEN.
45 C
46 C
47 C      NOTE. LSQR USES AN ITERATIVE METHOD TO APPROXIMATE THE SOLUTION.
48 C      THE NUMBER OF ITERATIONS REQUIRED TO REACH A CERTAIN ACCURACY
49 C      DEPENDS STRONGLY ON THE SCALING OF THE PROBLEM. POOR SCALING OF
50 C      THE ROWS OR COLUMNS OF A SHOULD THEREFORE BE AVOIDED WHERE
51 C      POSSIBLE.
52 C
53 C      FOR EXAMPLE, IN PROBLEM 1 THE SOLUTION IS UNALTERED BY
54 C      ROW-SCALING. IF A ROW OF A IS VERY SMALL OR LARGE COMPARED TO
55 C      THE OTHER ROWS OF A, THE CORRESPONDING ROW OF ( A B ) SHOULD
56 C      BE SCALED UP OR DOWN.
57 C
58 C      IN PROBLEMS 1 AND 2, THE SOLUTION X IS EASILY RECOVERED
59 C      FOLLOWING COLUMN-SCALING. IN THE ABSENCE OF BETTER INFORMATION,
60 C      THE NONZERO COLUMNS OF A SHOULD BE SCALED SO THAT THEY ALL HAVE
61 C      THE SAME EUCLIDEAN NORM (E.G. 1.0).
62 C
63 C      IN PROBLEM 3, THERE IS NO FREEDOM TO RE-SCALE IF DAMP IS
64 C      NONZERO. HOWEVER, THE VALUE OF DAMP SHOULD BE ASSIGNED ONLY
65 C      AFTER ATTENTION HAS BEEN PAID TO THE SCALING OF A.
66 C
67 C      THE PARAMETER DAMP IS INTENDED TO HELP REGULARIZE
68 C      ILL-CONDITIONED SYSTEMS, BY PREVENTING THE TRUE SOLUTION FROM
69 C      BEING VERY LARGE. ANOTHER AID TO REGULARIZATION IS PROVIDED BY
70 C      THE PARAMETER ACOND, WHICH MAY BE USED TO TERMINATE ITERATIONS
71 C      BEFORE THE COMPUTED SOLUTION BECOMES VERY LARGE.
72 C
73 C
74 C      NOTATION
75 C      -----
76 C
77 C      THE FOLLOWING QUANTITIES ARE USED IN DISCUSSING THE SUBROUTINE
78 C      PARAMETERS...
79 C
80 C      ABAR = ( A ),          BBAR = ( B )
81 C            ( DAMP*I )      ( 0 )
82 C

```

```

83 C      R      = B - A*X,          RBAR = BBAR - ABAR*X
84 C
85 C      RNORM   = SQRT( NORM(R)**2 + DAMP**2 * NORM(X)**2 )
86 C              = NORM( RBAR )
87 C
88 C      RELPR   = THE RELATIVE PRECISION OF FLOATING-POINT ARITHMETIC
89 C                  ON THE MACHINE BEING USED.  FOR EXAMPLE, ON THE IBM 370,
90 C                  RELPR IS ABOUT 1.0E-6 AND 1.0D-16 IN SINGLE AND DOUBLE
91 C                  PRECISION RESPECTIVELY.
92 C
93 C      LSQR MINIMIZES THE FUNCTION RNORM WITH RESPECT TO X.
94 C
95 C
96 C      PARAMETERS
97 C      -----
98 C
99 C      M      INPUT      THE NUMBER OF ROWS IN  A.
100 C
101 C      N      INPUT      THE NUMBER OF COLUMNS IN  A.
102 C
103 C      APROD   EXTERNAL   SEE ABOVE.
104 C
105 C      DAMP    INPUT      THE DAMPING PARAMETER FOR PROBLEM 3 ABOVE.
106 C                      (DAMP SHOULD BE 0.0 FOR PROBLEMS 1 AND 2.)
107 C                      IF THE SYSTEM A*X = B IS INCOMPATIBLE, VALUES
108 C                      OF DAMP IN THE RANGE 0 TO SQRT(RELPR)*NORM(A)
109 C                      WILL PROBABLY HAVE A NEGLIGIBLE EFFECT.
110 C                      LARGER VALUES OF DAMP WILL TEND TO DECREASE
111 C                      THE NORM OF X AND TO REDUCE THE NUMBER OF
112 C                      ITERATIONS REQUIRED BY LSQR.
113 C
114 C                      THE WORK PER ITERATION AND THE STORAGE NEEDED
115 C                      BY LSQR ARE THE SAME FOR ALL VALUES OF DAMP.
116 C
117 C      IA      INPUT      CONTAINS ROW INFORMATION OF          ARRAY  A.
118 C      JA      INPUT      CONTAINS COLUMN INFORMATION OF A ROW WITHIN  A.
119 C      AA      INPUT      THE  A  ARRAY.
120 C
121 C      NOTE.  LSQR DOES NOT EXPLICITLY USE THE PREVIOUS FOUR
122 C      PARAMETERS, BUT PASSES THEM TO SUBROUTINE APROD FOR
123 C      POSSIBLE USE AS WORKSPACE.  IF APROD DOES NOT NEED
124 C      IW OR RW, THE VALUES LENIW = 1 OR LENRW = 1 SHOULD
125 C      BE USED, AND THE ACTUAL PARAMETERS CORRESPONDING TO
126 C      IW OR RW MAY BE ANY CONVENIENT ARRAY OF SUITABLE TYPE.
127 C
128 C      U(M)    INPUT      THE RHS VECTOR B.  BEWARE THAT U IS
129 C                      OVER-WRITTEN BY LSQR.
130 C
131 C      V(N)    WORKSPACE
132 C      W(N)    WORKSPACE
133 C
134 C      X(N)    OUTPUT      RETURNS THE COMPUTED SOLUTION X.
135 C

```

```

136 C      SE(N)  OUTPUT  RETURNS STANDARD ERROR ESTIMATES FOR THE
137 C                                COMPONENTS OF X.  FOR EACH I, SE(I) IS SET
138 C                                TO THE VALUE RNORM * SQRT( SIGMA(I,I) / T ),
139 C                                WHERE SIGMA(I,I) IS AN ESTIMATE OF THE I-TH
140 C                                DIAGONAL OF THE INVERSE OF ABAR(TRANPOSE)*ABAR
141 C                                AND T = 1      IF M .LE. N,
142 C                                T = M - N  IF M .GT. N  AND  DAMP = 0,
143 C                                T = M      IF DAMP .NE. 0.
144 C
145 C      ATOL    INPUT   AN ESTIMATE OF THE RELATIVE ERROR IN THE DATA
146 C                                DEFINING THE MATRIX A.  FOR EXAMPLE,
147 C                                IF A IS ACCURATE TO ABOUT 6 DIGITS, SET
148 C                                ATOL = 1.0E-6 .
149 C
150 C      BTOL    INPUT   AN ESTIMATE OF THE RELATIVE ERROR IN THE DATA
151 C                                DEFINING THE RHS VECTOR B.  FOR EXAMPLE,
152 C                                IF B IS ACCURATE TO ABOUT 6 DIGITS, SET
153 C                                BTOL = 1.0E-6 .
154 C
155 C      CONLIM  INPUT   AN UPPER LIMIT ON COND(ABAR), THE APPARENT
156 C                                CONDITION NUMBER OF THE MATRIX ABAR.
157 C                                ITERATIONS WILL BE TERMINATED IF A COMPUTED
158 C                                ESTIMATE OF COND(ABAR) EXCEEDS CONLIM.
159 C                                THIS IS INTENDED TO PREVENT CERTAIN SMALL OR
160 C                                ZERO SINGULAR VALUES OF A OR ABAR FROM
161 C                                COMING INTO EFFECT AND CAUSING UNWANTED GROWTH
162 C                                IN THE COMPUTED SOLUTION.
163 C
164 C                                CONLIM AND DAMP MAY BE USED SEPARATELY OR
165 C                                TOGETHER TO REGULARIZE ILL-CONDITIONED SYSTEMS.
166 C
167 C                                NORMALLY, CONLIM SHOULD BE IN THE RANGE
168 C                                1000 TO 1/RELPR.
169 C                                SUGGESTED VALUE --
170 C                                CONLIM = 1/(100*RELPR) FOR COMPATIBLE SYSTEMS,
171 C                                CONLIM = 1/(10*SQRT(RELPR)) FOR LEAST SQUARES.
172 C
173 C                                NOTE. IF THE USER IS NOT CONCERNED ABOUT THE PARAMETERS
174 C                                ATOL, BTOL AND CONLIM, ANY OR ALL OF THEM MAY BE SET
175 C                                TO ZERO. THE EFFECT WILL BE THE SAME AS THE VALUES
176 C                                RELPR, RELPR AND 1/RELPR RESPECTIVELY.
177 C
178 C      ITNLIM  INPUT   AN UPPER LIMIT ON THE NUMBER OF ITERATIONS.
179 C                                SUGGESTED VALUE --
180 C                                ITNLIM = N/2      FOR WELL CONDITIONED SYSTEMS,
181 C                                ITNLIM = 4*N      OTHERWISE.
182 C
183 C      NOUT    INPUT   FILE NUMBER FOR PRINTER.  IF POSITIVE,
184 C                                A SUMMARY WILL BE PRINTED ON FILE NOUT.
185 C
186 C      ISTOP   OUTPUT  AN INTEGER GIVING THE REASON FOR TERMINATION...
187 C
188 C      0       X = 0 IS THE EXACT SOLUTION.

```

189	C		NO ITERATIONS WERE PERFORMED.
190	C		
191	C	1	THE EQUATIONS $A*X = B$ ARE PROBABLY
192	C		COMPATIBLE. $NORM(A*X - B)$ IS SUFFICIENTLY
193	C		SMALL, GIVEN THE VALUES OF ATOL AND BTOL.
194	C		
195	C	2	THE SYSTEM $A*X = B$ IS PROBABLY NOT
196	C		COMPATIBLE. A LEAST-SQUARES SOLUTION HAS
197	C		BEEN OBTAINED WHICH IS SUFFICIENTLY ACCURATE,
198	C		GIVEN THE VALUE OF ATOL.
199	C		
200	C	3	AN ESTIMATE OF $COND(ABAR)$ HAS EXCEEDED
201	C		CONLIM. THE SYSTEM $A*X = B$ APPEARS TO BE
202	C		ILL-CONDITIONED. OTHERWISE, THERE COULD BE AN
203	C		AN ERROR IN SUBROUTINE APROD.
204	C		
205	C	4	THE EQUATIONS $A*X = B$ ARE PROBABLY
206	C		COMPATIBLE. $NORM(A*X - B)$ IS AS SMALL AS
207	C		SEEMS REASONABLE ON THIS MACHINE.
208	C		
209	C	5	THE SYSTEM $A*X = B$ IS PROBABLY NOT
210	C		COMPATIBLE. A LEAST-SQUARES SOLUTION HAS
211	C		BEEN OBTAINED WHICH IS AS ACCURATE AS SEEMS
212	C		REASONABLE ON THIS MACHINE.
213	C		
214	C	6	$COND(ABAR)$ SEEMS TO BE SO LARGE THAT THERE IS
215	C		NOT MUCH POINT IN DOING FURTHER ITERATIONS,
216	C		GIVEN THE PRECISION OF THIS MACHINE.
217	C		THERE COULD BE AN ERROR IN SUBROUTINE APROD.
218	C		
219	C	7	THE ITERATION LIMIT ITNLIM WAS REACHED.
220	C		
221	C	ANORM OUTPUT	AN ESTIMATE OF THE FROBENIUS NORM OF ABAR.
222	C		THIS IS THE SQUARE-ROOT OF THE SUM OF SQUARES
223	C		OF THE ELEMENTS OF ABAR.
224	C		IF DAMP IS SMALL AND IF THE COLUMNS OF A
225	C		HAVE ALL BEEN SCALED TO HAVE LENGTH 1.0,
226	C		ANORM SHOULD INCREASE TO ROUGHLY $\sqrt{N}$.
227	C		A RADICALLY DIFFERENT VALUE FOR ANORM MAY
228	C		INDICATE AN ERROR IN SUBROUTINE APROD (THERE
229	C		MAY BE AN INCONSISTENCY BETWEEN MODES 1 AND 2).
230	C		
231	C	ACOND OUTPUT	AN ESTIMATE OF $COND(ABAR)$, THE CONDITION
232	C		NUMBER OF ABAR. A VERY HIGH VALUE OF ACOND
233	C		MAY AGAIN INDICATE AN ERROR IN APROD.
234	C		
235	C	RNORM OUTPUT	AN ESTIMATE OF THE FINAL VALUE OF $NORM(RBAR)$,
236	C		THE FUNCTION BEING MINIMIZED (SEE NOTATION
237	C		ABOVE). THIS WILL BE SMALL IF $A*X = B$ HAS
238	C		A SOLUTION.
239	C		
240	C	ARNORM OUTPUT	AN ESTIMATE OF THE FINAL VALUE OF
241	C		$NORM(ABAR(TRANSPOSE)*RBAR)$, THE NORM OF


```

242 C          THE RESIDUAL FOR THE USUAL NORMAL EQUATIONS.
243 C          THIS SHOULD BE SMALL IN ALL CASES. (ARNORM
244 C          WILL OFTEN BE SMALLER THAN THE TRUE VALUE
245 C          COMPUTED FROM THE OUTPUT VECTOR X.)
246 C
247 C  XNORM  OUTPUT  AN ESTIMATE OF THE NORM OF THE FINAL
248 C          SOLUTION VECTOR X.
249 C
250 C
251 C  SUBROUTINES AND FUNCTIONS USED
252 C  -----
253 C
254 C  USER      APROD
255 C  LSQR      NORMLZ
256 C  BLAS      SCOPY,SNRM2,SSCAL (SEE LAWSON ET AL. BELOW)
257 C          (SNRM2 IS USED ONLY IN NORMLZ)
258 C  FORTRAN   ABS,MOD,SQRT
259 C
260 C
261 C  PRECISION
262 C  -----
263 C
264 C  THE NUMBER OF ITERATIONS REQUIRED BY LSQR WILL USUALLY DECREASE
265 C  IF THE COMPUTATION IS PERFORMED IN HIGHER PRECISION. TO CONVERT
266 C  LSQR AND NORMLZ BETWEEN SINGLE- AND DOUBLE-PRECISION, CHANGE
267 C  THE WORDS
268 C          SCOPY, SNRM2, SSCAL
269 C          ABS, REAL, SQRT
270 C  TO THE APPROPRIATE BLAS AND FORTRAN EQUIVALENTS.
271 C
272 C
273 C  REFERENCES
274 C  -----
275 C
276 C  PAIGE, C.C. AND SAUNDERS, M.A. LSQRØD AN ALGORITHM FOR SPARSE
277 C  LINEAR EQUATIONS AND SPARSE LEAST SQUARES.
278 C  ACM TRANSACTIONS ON MATHEMATICAL SOFTWARE 8, 1 (MARCH 1982).
279 C
280 C  LAWSON, C.L., HANSON, R.J., KINCAID, D.R. AND KROGH, F.T.
281 C  BASIC LINEAR ALGEBRA SUBPROGRAMS FOR FORTRAN USAGE.
282 C  ACM TRANSACTIONS ON MATHEMATICAL SOFTWARE 5, 3 (SEPT 1979),
283 C  308-323 AND 324-325.
284 C
285 C
286 C  LSQR.      THIS VERSION DATED 22 FEBRUARY 1982.
287 C  -----
288 C
289 C  FUNCTIONS AND LOCAL VARIABLES
290 C
291 C  INTEGER   I,ITN,MOD,NCONV,NSTOP
292 C  REAL      ABS,SQRT
293 C  REAL      ALFA,BBNORM,BETA,BNORM,
294 C  1         CS,CS1,CS2,CTOL,DAMPSQ,DDNORM,DELTA,

```



```

295      2      GAMMA,GAMBAR,ONE,PHI,PHIBAR,PSI,
296      3      RES1,RES2,RHO,RHOBAR,RHBAR1,RHBAR2,RHS,RTOL,
297      4      SN,SN1,SN2,T,TAU,TEST1,TEST2,TEST3,
298      5      THETA,T1,T2,T3,XXNORM,Z,ZBAR,ZERO
299  C
300  C
301  C      INITIALIZE.
302  C
303      IF (NOUT .GT. 0)
304      1  WRITE(NOUT, 1000) M,N,DAMP,ATOL,CONCLIM,BTOL,ITNLM
305      ZERO   = 0.0
306      ONE    = 1.0
307      CTOL   = ZERO
308      IF (CONCLIM .GT. ZERO) CTOL = ONE/CONCLIM
309      DAMPSQ  = DAMP**2
310      ANORM   = ZERO
311      ACOND   = ZERO
312      BBNORM  = ZERO
313      DDNORM  = ZERO
314      RES2    = ZERO
315      XNORM   = ZERO
316      XXNORM  = ZERO
317      CS2     = -ONE
318      SN2     = ZERO
319      Z       = ZERO
320      ITN     = 0
321      ISTOP   = 0
322      NSTOP   = 0
323  C
324      DO 10 I = 1, N
325          V(I) = ZERO
326          X(I) = ZERO
327          SE(I) = ZERO
328      10 CONTINUE
329  C
330  C      SET UP THE FIRST VECTORS FOR THE BIDIAGONALIZATION.
331  C      THESE SATISFY  BETA*U = B,  ALFA*V = A(TRANPOSE)*U.
332  C
333      CALL NORMLZ( M,U,BETA )
334      CALL APROD ( 2,M,N,V,U,  IA,JA,AA )
335      CALL NORMLZ( N,V,ALFA )
336      CALL SCOPY ( N,V,1,W,1 )
337  C
338      RHOBAR = ALFA
339      PHIBAR = BETA
340      BNORM  = BETA
341      RNORM  = BETA
342      ARNORM = ALFA*BETA
343      IF (ARNORM .LE. ZERO) GO TO 800
344      IF (NOUT .LE. 0 ) GO TO 100
345      IF (DAMPSQ .LE. ZERO) WRITE(NOUT, 1200)
346      IF (DAMPSQ .GT. ZERO) WRITE(NOUT, 1300)
347      TEST1 = ONE

```

```

348      TEST2 = ALFA/BETA
349      WRITE(NOUT, 1500) ITN,X(1),RNCRM,TEST1,TEST2
350      WRITE(NOUT, 1600)
351  C
352  C -----
353  C MAIN ITERATION LOOP.
354  C -----
355      100 ITN = ITN + 1
356  C
357  C PERFORM THE NEXT STEP OF THE BIDIAGONALIZATION TO OBTAIN THE
358  C NEXT BETA, U, ALFA, V. THESE SATISFY THE RELATIONS
359  C      BETA*U = A*V - ALFA*U,
360  C      ALFA*V = A(TRANSPPOSE)*U - BETA*V.
361  C
362  C CALL SSCAL ( M,(-ALFA),U,1 )
363  C CALL APROD ( 1,M,N,V,U, IA,JA,AA )
364  C CALL NORMLZ( M,U,BETA )
365  C BBNORM = BBNORM + ALFA**2 + BETA**2 + DAMPSQ
366  C CALL SSCAL ( N,(-BETA),V,1 )
367  C CALL APROD ( 2,M,N,V,U, IA,JA,AA )
368  C CALL NORMLZ( N,V,ALFA )
369  C
370  C
371  C USE A PLANE ROTATION TO ELIMINATE THE DAMPING PARAMETER.
372  C THIS ALTERS THE DIAGONAL (RHOBAR) OF THE LOWER-BIDIAGONAL MATRIX.
373  C
374  C RHBAR2 = RHOBAR**2 + DAMPSQ
375  C RHBAR1 = SQRT(RHBAR2)
376  C CS1 = RHOBAR/RHBAR1
377  C SN1 = DAMP/RHBAR1
378  C PSI = SN1*PHIBAR
379  C PHIBAR = CS1*PHIBAR
380  C
381  C
382  C USE A PLANE ROTATION TO ELIMINATE THE SUBDIAGONAL ELEMENT (BETA)
383  C OF THE LOWER-BIDIAGONAL MATRIX, GIVING AN UPPER-BIDIAGONAL MATRIX.
384  C
385  C RHO = SQRT(RHBAR2 + BETA**2)
386  C CS = RHBAR1/RHO
387  C SN = BETA/RHO
388  C THETA = SN*ALFA
389  C RHOBAR = -CS*ALFA
390  C PHI = CS*PHIBAR
391  C PHIBAR = SN*PHIBAR
392  C TAU = SN*PHI
393  C
394  C
395  C UPDATE X, W AND THE STANDARD ERROR ESTIMATES.
396  C
397  C T1 = PHI/RHO
398  C T2 = -THETA/RHO
399  C T3 = ONE/RHO
400  C

```

```

401      DO 200 I = 1, N
402          T      = W(I)
403          X(I)   = T1*T + X(I)
404          W(I)   = T2*T + V(I)
405          T      = (T3*T)**2
406          SE(I)  = T + SE(I)
407          DDNORM = T + DDNORM
408      200 CONTINUE
409      C
410      C
411      C      USE A PLANE ROTATION ON THE RIGHT TO ELIMINATE THE
412      C      SUPER-DIAGONAL ELEMENT (THETA) OF THE UPPER-BIDIAGONAL MATRIX.
413      C      THEN USE THE RESULT TO ESTIMATE  NORM(X).
414      C
415      DELTA = SN2*RHO
416      GAMBAR = -CS2*RHO
417      RHS = PHI - DELTA*Z
418      ZBAR = RHS/GAMBAR
419      XNORM = SQRT(XNORM + ZBAR**2)
420      GAMMA = SQRT(GAMBAR**2 + THETA**2)
421      CS2 = GAMBAR/GAMMA
422      SN2 = THETA/GAMMA
423      Z = RHS/GAMMA
424      XXNORM = XXNORM + Z**2
425      C
426      C
427      C      TEST FOR CONVERGENCE.
428      C      FIRST, ESTIMATE THE NORM AND CONDITION OF THE MATRIX ABAR,
429      C      AND THE NORMS OF RBAR AND ABAR(TRANSPPOSE)*RBAR.
430      C
431      ANORM = SQRT(BBNORM)
432      ACOND = ANORM*SQRT(DDNORM)
433      RES1 = PHIBAR**2
434      RES2 = RES2 + PSI**2
435      RNORM = SQRT(RES1 + RES2)
436      ARNORM = ALFA*ABS(TAU)
437      C
438      C      NOW USE THESE NORMS TO ESTIMATE CERTAIN OTHER QUANTITIES,
439      C      SOME OF WHICH WILL BE SMALL NEAR A SOLUTION.
440      C
441      TEST1 = RNORM/BNORM
442      TEST2 = ARNORM/(ANORM*RNORM)
443      TEST3 = ONE/ACOND
444      T1 = TEST1/(ONE + ANORM*XNORM/BNORM)
445      RTOL = BTOL + ATOL*ANORM*XNORM/BNORM
446      C
447      C      THE FOLLOWING TESTS GUARD AGAINST EXTREMELY SMALL VALUES OF
448      C      ATOL, BTOL OR CTOL. (THE USER MAY HAVE SET ANY OR ALL OF
449      C      THE PARAMETERS ATOL, BTOL, CONLIM TO ZERO.)
450      C      THE EFFECT IS EQUIVALENT TO THE NORMAL TESTS USING
451      C      ATOL = RELPR, BTOL = RELPR, CONLIM = 1/RELPR.
452      C
453      T3 = ONE + TEST3

```

```

454      T2 = ONE + TEST2
455      T1 = ONE + T1
456      IF (ITN .GE. ITNLIM) ISTOP = 7
457      IF (T3 .LE. ONE ) ISTOP = 6
458      IF (T2 .LE. ONE ) ISTOP = 5
459      IF (T1 .LE. ONE ) ISTOP = 4
460 C
461 C      ALLOW FOR TOLERANCES SET BY THE USER.
462 C
463      IF (TEST3 .LE. CTOL) ISTOP = 3
464      IF (TEST2 .LE. ATOL) ISTOP = 2
465      IF (TEST1 .LE. RTOL) ISTOP = 1
466 C      =====
467 C
468 C      SEE IF IT IS TIME TO PRINT SOMETHING.
469 C
470      IF (NOUT .LE. 0) GO TO 600
471      IF (M.LE.40 .OR. N.LE.40) GO TO 400
472      IF (ITN .LE. 10)          GO TO 400
473      IF (ITN .GE. ITNLIM-10)   GO TO 400
474      IF (MOD(ITN,10) .EQ. 0)   GO TO 400
475      IF (TEST3 .LE. 2.0*CTOL) GO TO 400
476      IF (TEST2 .LE. 10.0*ATOL) GO TO 400
477      IF (TEST1 .LE. 10.0*RTOL) GO TO 400
478      GO TO 600
479 C
480 C      PRINT A LINE FOR THIS ITERATION.
481 C
482      400 WRITE(NOUT, 1600) ITN,X(1),RNORM,TEST1,TEST2,ANORM,ACOND
483      IF (MOD(ITN,10) .EQ. 0) WRITE(NOUT, 1600)
484 C      =====
485 C
486 C      STOP IF APPROPRIATE.
487 C      THE CONVERGENCE CRITERIA ARE REQUIRED TO BE MET ON NCONV
488 C      CONSECUTIVE ITERATIONS, WHERE NCONV IS SET BELOW.
489 C      SUGGESTED VALUE -- NCONV = 1, 2 OR 3.
490 C
491      600 IF (ISTOP .EQ. 0) NSTOP = 0
492      IF (ISTOP .EQ. 0) GO TO 100
493      NCONV = 1
494      NSTOP = NSTOP + 1
495      IF (NSTOP .LT. NCONV .AND. ITN .LT. ITNLIM) ISTOP = 0
496      IF (ISTOP .EQ. 0) GO TO 100
497 C      -----
498 C      END OF ITERATION LOOP.
499 C      -----
500 C
501 C
502 C      FINISH OFF THE STANDARD ERROR ESTIMATES.
503 C
504      T = ONE
505      IF (M .GT. N) T = M - N
506      IF (DAMPSQ .GT. ZERO) T = M

```

```

507      T = RNORM/SQRT(T)
508 C
509      DO 700 I = 1, N
510          SE(I) = T*SQRT(SE(I))
511      700 CONTINUE
512 C
513 C      PRINT THE STOPPING CONDITION.
514 C
515      800 IF (NOUT .LE. 0) GO TO 900
516          WRITE(NOUT, 1900) ITN,ISTOP
517          IF (ISTOP .EQ. 0) WRITE(NOUT, 2000)
518          IF (ISTOP .EQ. 1) WRITE(NOUT, 2100)
519          IF (ISTOP .EQ. 2) WRITE(NOUT, 2200)
520          IF (ISTOP .EQ. 3) WRITE(NOUT, 2300)
521          IF (ISTOP .EQ. 4) WRITE(NOUT, 2400)
522          IF (ISTOP .EQ. 5) WRITE(NOUT, 2500)
523          IF (ISTOP .EQ. 6) WRITE(NOUT, 2600)
524          IF (ISTOP .EQ. 7) WRITE(NOUT, 2700)
525      900 RETURN
526 C      -----
527 C
528      1000 FORMAT(
529          1 // 25X, 46HLSQR -- LEAST-SQUARES SOLUTION OF A*X = B
530          2 // 25X, 18HTHE MATRIX A HAS, I6, 11H ROWS AND, I6, 5H COLS
531          3 / 25X, 36HTHE DAMPING PARAMETER IS DAMP =, 1PE10.2
532          4 // 25X, 8HATOL =, 1PE10.2, 10X, 8HCONLM =, 1PE10.2
533          5 / 25X, 8HBTOL =, 1PE10.2, 10X, 8HITNLM =, I10)
534      1200 FORMAT(/ 3X, 3HITN, 9X, 4HX(1), 14X, 8HFUNCTION, 7X,
535          1 45HCOMPATIBLE INCOMPATIBLE NORM(A) COND(A) /)
536      1300 FORMAT(/ 3X, 3HITN, 9X, 4HX(1), 14X, 8HFUNCTION, 7X,
537          1 45HCOMPATIBLE INCOMPATIBLE NORM(ABAR) COND(ABAR) /)
538      1500 FORMAT(I6, 1PE20.10, 1PE19.10, 1P2E13.3, 1P2E11.2)
539      1600 FORMAT(1X)
540      1900 FORMAT(/ 20H NO. OF ITERATIONS =, I6,
541          1 8X, 21H STOPPING CONDITION =, I3)
542      2000 FORMAT(/ 52H THE EXACT SOLUTION IS X = 0. )
543      2100 FORMAT(/ 52H A*X - B IS SMALL ENOUGH, GIVEN ATOL, BTOL )
544      2200 FORMAT(/ 52H THE LEAST-SQRS SOLN IS GOOD ENOUGH, GIVEN ATOL )
545      2300 FORMAT(/ 52H THE ESTIMATE OF COND(ABAR) HAS EXCEEDED CONLM )
546      2400 FORMAT(/ 52H A*X - B IS SMALL ENOUGH FOR THIS MACHINE )
547      2500 FORMAT(/ 52H THE LEAST-SQRS SOLN IS GOOD ENOUGH FOR THIS MACHINE)
548      2600 FORMAT(/ 52H COND(ABAR) SEEMS TO BE TOO LARGE FOR THIS MACHINE)
549      2700 FORMAT(/ 52H THE ITERATION LIMIT HAS BEEN REACHED )
550 C      END OF LSQR
551      END
552 C      -----
553      SUBROUTINE NORMLZ( N,X,BETA )
554          INTEGER N
555          REAL X(N),BETA
556 C
557 C      NORMLZ IS REQUIRED BY SUBROUTINE LSQR. IT COMPUTES THE
558 C      EUCLIDEAN NORM OF X AND RETURNS THE VALUE IN BETA.
559 C      IF X IS NONZERO, IT IS SCALED SO THAT NORM(X) = 1.

```



```

560 C
561 C   FUNCTIONS AND SUBROUTINES
562 C
563 C   BLAS       SNRM2,SSCAL
564 C
565 C   REAL       ONE,SNRM2,ZERO
566 C
567 C
568 C   ZERO = 0.0
569 C   ONE  = 1.0
570 C   BETA = SNRM2( N,X,1 )
571 C   IF (BETA .GT. ZERO) CALL SSCAL( N,(ONE/BETA),X,1 )
572 C   RETURN
573 C
574 C   END OF NORMLZ
575 C   END

```

6.3.8 SQRTT.FOR

```
1      function sqrtt (z)                ! assure proper branch
2      complex sqrtt, z, cmplx
3      data pi / 3.1415926E0 /
4
5      x = real (z)
6      y = aimag (z)
7      call polar (x,y,r,a,1)            ! [0,2)
8      if (r.eq.0.0) then
9          sqrtt = cmplx (0.0, 0.0)
10     else
11         r = sqrt (r)
12         a = a*pi*0.5                    ! [0, pi)
13         sqrtt = cmplx (r*cos(a), r*sin(a))
14     end if
15     return
16 end
```

6.3.9 POLAR.FOR

```

1  c-----
2      subroutine polar (x, y, r, a, icas)
3  c      given: x,y
4  c      discern: r,a
5  c      where: r>0, x=r*cos(a*pi), y=r*sin(a*pi)
6  c      case 1: a ' [ 0, 2)
7  c              2: a ' (-1, 1]
8  c              3: a ' [ 0, 2*pi)          ! radians
9  c              4: a ' [ 0, 360)          ! degrees
10
11      data pi / 3.14159265E0 /
12
13      if (y .eq. 0.0) then                ! x axis
14          if (x .lt. 0.0) then
15              a = 1.0
16              r = -x
17          else
18              a = 0.0
19              r = x
20          end if
21          goto 1
22      end if
23      if (x .eq. 0.0) then                ! y axis
24          if (y .lt. 0.0) then
25              a = 1.5
26              r = -y
27          else
28              a = 0.5
29              r = y
30          end if
31          goto 1
32      end if
33      xx = abs (x)
34      yy = abs (y)
35      if (xx .lt. yy) then
36          a = x/y                          ! ratio < 1
37          r = yy * sqrt (a*a+1.0)
38          a = 0.5 - atan (a) /pi          ! top
39          if (y .lt. 0.0) a=a+1.0         ! bottom
40      else
41          a = y/x                          ! ratio < 1
42          r = xx * sqrt (a*a+1.0)
43          a = atan (a) /pi
44          if (x .lt. 0.0) then            ! lhs
45              a = a+1.0
46          else if (y .lt. 0.0) then
47              a = a+2.0                  ! rhs
48          end if
49      end if
50

```

```

51      1 if (icase .eq. 1) return
52        if (icase .eq. 2) then
53          if (a .gt. 1.0) a=a-2.0
54          return
55        end if
56        if (icase .eq. 3) then          ! radians
57          a = a*pi
58        else                            ! degrees
59          a = a*180.0
60        end if
61
62      return
63    end

```

6.3.10 IINDEX.FOR

```

1  c      Discern the sequential index (k) for the (i,j) matrix element,
2  c      where the matrix is symmetric,  a(i,j) = a(j,i) = a(k),
3  c      but where only the upper/lower triangle is stored,  k=k(i,j).
4  c      N = size of the square matrix, i.e.,  A = a(i,j)  is NxN.
5  c      L = indicates the storage format, 1-4.
6
7  function iindex (l,n,i,j)
8  integer iindex, l,n,i,j
9
10     if (l.lt.1 .or. n.lt.1 .or. i.lt.1 .or. j.lt.1 .or.
11  &      l.gt.6 .or.          i.gt.n .or. j.gt.n ) then
12         call exit (2)          ! 2=error, 4=severe error
13     end if
14
15     mn = min (i,j)
16     mx = max (i,j)
17     goto (1,2,3,4,5,6), l
18
19  c      Symmetric Matix -----
20
21  c      Lower triangular matrix, j<=i, stored column by column.
22  1 iindex = mx + ((n+n-mn)*(mn-1))/2
23     return
24
25  c      Lower triangular matrix, j<=i, stored row by row.
26  2 iindex = mn + ((mx-1)*mx)/2
27     return
28
29  c      Upper triangular matrix, i<=j, stored column by column.
30  3 iindex = mn + ((mx-1)*mx)/2
31     return
32
33  c      Upper triangular matrix, i<=j, stored row by row.
34  4 iindex = mx + ((n+n-mn)*(mn-1))/2
35     return
36
37  c      Asymmetric Matrix -----
38
39  c      Full matrix, stored column by column.
40  5 iindex = i + (j-1)*n
41     return
42
43  c      Full matrix, stored row by row.
44  6 iindex = j + (i-1)*n
45     return
46
47     end

```


6.3.11 ISTE.FOR

```
1      function istance (i)          ! dummy argument
2      integer istance, iftime, i, it
3      logical first
4      data    first /.true./
5
6      entry iftime (i)
7      if (first) then              ! initial
8          first = .false.
9          call times (-1,it)       ! initialize cpu clock
10     end if
11     call times (1,it)             ! query elapsed cpu time (centi-seconds)
12     istance = it*10              ! milli-seconds
13     return
14     end
```

6.3.12 TIMES.FOR

```

1      subroutine times (is, it)
2      include 'sys$library:libdef.for'
3      include 'sys$library:sigdef.for'
4  c*   include 'sys$library:mthdef.for'
5  c*   include 'sys$library:fordef.for'
6
7      parameter (io=6, nh=2)
8      integer*4  handle(nh), status
9      save      handle
10
11  c-----
12  c      This routine maintains or keeps track of several distinct
13  c      or separate and independent clocks.
14  c      Each clock is equivalent to any other clock,
15  c      i.e., among themselves.
16  c      The number of clocks is restricted by the magnitude
17  c      or dimension of the array, "handle", i.e., "nh".
18  c      The clocks are indexed by the magnitude of "is" = |is|.
19  c      A clock is initialized whenever "is" is negative;
20  c      all clocks are initialized whenever "is" is zero.
21  c      Time displacements or intervals, "it", are:
22  c      a)  evaluated whenever "is" is positive
23  c      b)  expressed in units of:  centi-seconds
24  c-----
25
26      if (is.eq.0) then                ! initialize all clocks
27          do i=1,nh                    ! scan distinct clocks
28              status = lib$init_timer (handle(i))
29              if (status.ne.ss$_normal) then
30                  write (io,6)
31                  stop
32              end if
33          end do
34          return
35      end if
36
37      if (iabs(is).gt.nh) then          ! nonexisting clock
38          write (io,8) is
39          stop
40      end if
41
42      if (is.lt.0) then                ! initialize, clock # |is|.
43          status = lib$init_timer (handle(-is))
44          if (status.eq.ss$_normal) return
45          write (io,6)
46          stop
47      else                             ! elapsed time, clock # (is).
48          status = lib$stat_timer (2,it,handle(is))
49          if (status.eq.ss$_normal) return
50          write (io,7)

```

```
51         stop
52     end if
53
54     6 format (' times, error: clock initalization problem.')
55     7 format (' times, error: clock evaluation problem.')
56     8 format (' times, error: using non-existing clock #', i2)
57     end
```

6.3.13 LJCHAR.FOR

```
1  c -----
2  c Left-justify and compress a character string
3  c by removing blank characters from the string.
4  c -----
5  subroutine ljchar (c)
6  character a, c*(*)
7
8  l = len (c)          ! length, number of characters in string
9  i = index (c, ' ')   ! locate first occurrence of blank character
10 if (i.eq.0 .or. i.eq.1) return
11
12 ii = i+1             ! index of next character
13 do j=ii,l            ! scan rightmost part of string
14   a = c(j:j)         ! extract next character
15   if (a.ne.' ') then
16     c(i:i) = a        ! fill on left
17     c(j:j) = ' '      ! fill on right
18     i = i+1           ! update index
19   end if
20 end do
21 return
22 end
```

6.3.14 HHLINE.FOR

```
1      subroutine hhlne (idat, iout)  ! used only by:  INPDAT
2
3      character*50  dlimit, hyphen  ! convenience
4      data hyphen/'-----',/
5
6      read (idat,2) dlimit
7      if (dlimit .eq. hyphen) then
8          write (iout,3) dlimit
9      else
10         write (iout,4) dlimit, hyphen
11         stop
12     end if
13     return
14
15     2 format (a)
16     3 format (1x, a)
17     4 format (/ ' ... oops,  inadequate delimiter'
18     &        /' read:', a          /' want:', a)
19     end
```


6.4 Dielectric Functions, Effective Media

6.4.1 DIEFCN.FOR

```
1  c      Evaluate:      dielectric function      of mixture.
2  c      Consider:
3  c          1)      volume fractions, effective medium approximation
4  c          2)      structure fractions, depolarization factors ... (not yet)
5  c          3)      mixture parameters
6  c          4)      ambient parameters
7  c      -----
8
9      subroutine diefcn (imbien, imixtr,
10 &                      anglei, wavlen, dielec,
11 &                      dielew, dielff, dielpp, dielpa)
12
13      complex  dielec, dielew, dielff(1), dielpp(1), dielpa(1)
14
15      include 'iounit.'
16      include 'defnit.'
17      include 'filmmn.'
18      include 'handyy.'                ! pi
19
20      complex  diel(nlmnts), diew(nlmnts), ss(nlmnts)
21      integer  iipa(nparms), iipp(nparms)
22      real     rrpa(nparms), rrup(nparms)
23      integer  llpa(nparms), llpp(nparms)
24      parameter (klmnts=5)             ! convenience
25      complex  ddpa(nparms,klmnts), ddpp(nparms,klmnts) ! (nparms,nlmnts)
26
27
28      mm = mmixtr+imbien                ! offset, ambient
29
30      mipa = miparm(mm)
31      kipa = kiparm(mm)
32      if (mipa.ne.0) then                ! ambient parameters
33          ki = kipa
34          do m=1,mipa
35              ki = ki+1
36              ip = jiparm(ki)
37              iipa(m) = iiparm(ip)
38          end do
39      end if
40
41      mrpa = mrparm(mm)
42      krpa = krparm(mm)
43      if (mrpa.ne.0) then                ! ambient parameters
44          kr = krpa
45          do m=1,mrpa
46              kr = kr+1
47              ip = jrparm(kr)
48              rrpa(m) = rrparm(ip)
```

```

49         llpa(m) = lrparm(ip)
50     end do
51 end if
52
53 mipp = miparm(imixtr)
54 kipp = kiparm(imixtr)           ! offset ---> jiparm ---> iiparm
55 if (mipp.ne.0) then
56     ki = kipp
57     do m=1,mipp
58         ki = ki+1
59         ip = jiparm(ki)
60         iipp(m) = iiparm(ip)
61     end do
62 end if
63
64 mrpp = mrparm(imixtr)
65 krpp = krparm(imixtr)           ! offset ---> jrparm ---> rrparm
66 if (mrpp.ne.0) then
67     kr = krpp
68     do m=1,mrpp
69         kr = kr+1
70         ip = jrparm(kr)
71         rrpp(m) = rrparm(ip)
72         llpp(m) = lrparm(ip)
73     end do
74 end if
75
76 mmlmn = mmlmnt(imixtr)           ! quantity of elements in mixture
77 kklmn = kklmnt(imixtr)           ! offset ---> iilmnt
78 c =====
79 if (mmlmn.ne.0) then             ! volume fractions
80     if (mmlmn.gt. klmnts) then    ! insure sufficient workspace
81         write (iout,111) mmlmn
82         stop
83     end if
84
85     kk = kklmn
86     do i=1,mmlmn                 ! scan elements
87         kk = kk+1
88         lmnt = iilmnt(kk)         ! specific element
89 c         frac = fflmnt(kk)       ! volume fraction
90
91         if (mrpp.ne.0) then       ! initialize
92             do j=1,mrpp
93                 ddpp(j,i) = cmplx (0.0, 0.0)
94             end do
95         end if
96         if (mrpa.ne.0) then       ! initialize
97             do j=1,mrpa
98                 ddpa(j,i) = cmplx (0.0, 0.0)
99             end do
100         end if
101

```

```

102      call dielmn (lmnt, anglei, wavlen, diel(i), dielw(i),
103      &          mipp,iipp, mrpp,rrpp,llpp, ddpp(1,i),
104      &          mipa,iipa, mrpa,rrpa,llpa, ddpa(1,i) )
105      end do
106
107      kk = kklmn+1      ! locate volume fractions
108      call dieema (mmlmn, fflmnt(kk), diel, dielw, dielff,
109      &          dielec, dielew,          ss )
110
111      if (mrpp .ne. 0) then
112          do j=1,mrpp
113              do i=1,mmlmn
114                  ss(i) = ddpp(j,i)
115              end do
116              call diemad (mmlmn, fflmnt(kk), diel, ss,
117      &          dielec, dielpj(j)          )
118          end do
119      end if
120      if (mrpa .ne. 0) then
121          do j=1,mrpa
122              do i=1,mmlmn
123                  ss(i) = ddpa(j,i)
124              end do
125              call diemad (mmlmn, fflmnt(kk), diel, ss,
126      &          dielec, dielpa(j)          )
127          end do
128      end if
129
130      end if      ! volume fractions
131  c  =====
132  c  Determine:  d (dielectric function(w)) /d (mixture parameters)
133
134  c*  if (mrpp.ne.0) then      ! mixture parameters
135  c*      kr = krpp
136  c*      do irp=1,mrpp
137  c*          kr = kr+1
138  c*          dielpj(irp) = 0.0
139  c*      end do
140  c*      dielec =      ... when ever necessary
141  c*      dielew =      ... when ever necessary
142  c*  end if
143  c  =====
144  c  Determine:  d (dielectric function(w)) /d (ambient parameters)
145
146  c*  if (mrpa.ne.0) then      ! ambient parameters
147  c*      kr = krpa
148  c*      do irp=1,mrpa
149  c*          kr = kr+1
150  c*          dielpa(irp) = 0.0
151  c*      end do
152  c*      dielec =      ... when ever necessary
153  c*      dielew =      ... when ever necessary
154  c*  end if

```

```

155 c      =====
156
157         return
158
159     111 format (' diefcn,      increase the allocation size '
160               &          '/'      of the second index of arrays:'
161               &          '/'      ddpp, ddpa.          '
162               &          '/'      to:  ', i5              )
163
164         end

```

6.4.2 DIEEMA.FOR

```

1  c -----
2  c Evaluate:      dielectric function  of a mixture
3  c   within:      the effective medium approximation
4  c   Method:      Newton iteration
5  c -----
6
7  subroutine dieema (mlmnt, frac, diel, diew, dief,
8  *                  dielec, dielew,          ss)
9
10 real      frac(mlmnt)
11 complex    diel(mlmnt), diew(mlmnt), dief(mlmnt)
12 complex    dielec, dielew
13 complex    ss(mlmnt)                ! workspace
14
15 complex    cmplx
16 complex    ss1, ss2, step, denom
17 complex    dies, died, fracc, third, one, zero
18
19 include 'iounit.'                  ! iout
20
21
22 third = cmplx (1.0/3.0, 0.0)
23 one   = cmplx (1.0, 0.0)
24 zero  = cmplx (0.0, 0.0)
25 ss1   = zero                        ! initialize
26 ss2   = zero
27
28 do i=1,mlmnt
29     fracc = cmplx (frac(i), 0.0)    ! volume fraction
30     dies  = diel(i)                 ! dielectric function
31     ss(i) = fracc*dies               ! convenience
32     ss1 = ss1+fracc*dies             ! shielding minimum
33     ss2 = ss2+fracc/dies             ! shielding maximum
34 end do
35
36 ss2 = one/ss2
37 dielec = (ss1+ss1+ss2)*third        ! estimate EMA
38
39 if (mlmnt.eq.1) goto 2
40 c -----
41 c Newton iteration
42
43 kt = 0
44 1 kt = kt+1                          ! iteration count
45     dies = zero                      ! residual, Q
46     died = zero                      ! gradient, dQ
47     do i=1,mlmnt
48         denom = diel(i) + dielec+dielec
49         step = ss(i)/denom           ! convenience
50         dies = dies+step             ! f(x)

```

```

51      died = died-step/denom          ! f'(x) /2
52      end do
53      dies = dies-third              ! Q = f(x) - f(root)
54      died = died+died              ! dQ = df/dx
55      step = -dies/died              ! Newton step
56
57      sx = real (step)
58      sy = aimag (step)
59      dx = real (dielec)
60      dy = aimag (dielec)
61      call polar (sx,sy, sr,sa, 1)    ! [0,2)
62      call polar (dx,dy, dr,da, 1)    ! [0,2)
63
64      if (kt .eq. 200) then           ! slow convergence
65          write (iout,101) kt, dies, step, dielec
66          stop
67      end if
68
69      if (sr .gt. 0.1*dr) then        ! limit stepsize
70          scal = 0.1*dr/sr
71          dielec = dielec + step*cmlpx (scal, 0.0)
72          goto 1
73      else
74          dielec = dielec + step      ! update solution
75          if (sr .ge. dr*1.0E-6) goto 1 ! test convergence
76      end if
77 c -----
78 c Convergence achieved.
79 c Evaluate:      (d/dw) (dielectric function EMA)
80 c and:          (d/df) (dielectric function EMA)
81
82 2 continue
83      dies = zero
84      died = zero
85      do i=1,mlmnt                ! fractions
86          denom = diel(i) + dielec+dielec
87          dief(i) = diel(i)/denom    ! df, convenience
88          denom = denom*denom
89          fracc = cmlpx (frac(i), 0.0)
90          dies = dies + ss(i) /denom ! de
91          died = died + diel(i)*fracc/denom ! dw
92      end do
93      dielew = dielec*(died/dies)    ! de/dw
94      dies = dies+dies
95      do i=1,mlmnt
96          dief(i) = dief(i)/dies    ! de/df
97      end do
98
99      return
100
101 101 format (/ ' dieEMA, slow convergence or divergence, '
102      &      /' iteration ' ', i5
103      &      /' residual ' ', 1p2e15.6

```



```
104      &      /'      Newton step - ',      2e15.6
105      &      /'      dielec - ',      2e15.6 )
106
107      end
```

6.4.3 DIEMAD.FOR

```
1  c      Evaluate:      dielectric function partial derivatives
2  c      within:       the effective medium approximation
3  c      -----
4
5      subroutine diemad (mlmnt, frac, diel, diew,
6      &                  dielec, dielew)
7
8      real      frac(mlmnt)
9      complex   diel(mlmnt), diew(mlmnt), dielec, dielew
10     complex   cmplx
11     complex   dies, died, fracc, denom
12
13     dies = cmplx (0.0, 0.0)
14     died = cmplx (0.0, 0.0)
15     do i=1,mlmnt                                ! fractions
16         denom = diel(i) + dielec+dielec
17         denom = denom*denom
18         fracc = cmplx (frac(i), 0.0)
19         dies = dies + diel(i)*fracc/denom        ! de
20         died = died + diew(i)*fracc/denom        ! dw
21     end do
22     dielew = dielec*(died/dies)                  ! de/dw
23
24     return
25     end
```

6.4.4 DIELMN.FOR

```

1      subroutine dielmn (lmnt,
2      &                  anglei, wavlen, dielec, dielew,
3      &                  mipp,iipp, mrpp,rrpp,llpp, ddpp,      ! mixture
4      &                  mipa,iipa, mrpa,rrpa,llpa, ddpa)      ! ambient
5
6      integer  iipa(1), iipp(1)
7      real     rrpa(1), rrpp(1)
8      integer  llpa(1), llpp(1)
9      complex  ddpa(1), ddpp(1), dielec, dielew
10
11      include 'iounit.'
12      include 'defnit.'
13
14
15      if (lmnt.lt.1 .or. lmnt.gt.nlmnts) then
16          write (iout,102) lmnt, nlmnts
17          stop
18      end if
19
20      goto ( 1, 2, 3, 4, 5, 6, 7, 8, 9, 10,
21      &      11, 12, 13, 14, 15, 16, 17, 18, 19, 20 ), lmnt
22      write (iout,103)
23      stop
24
25  c -----
26  1 continue      ! vacuum
27      call diel01 (anglei, wavlen, dielec, dielew,
28      &            mipp,iipp, mrpp,rrpp,llpp, ddpp,
29      &            mipa,iipa, mrpa,rrpa,llpa, ddpa)
30      goto 101
31  c -----
32  2 continue      ! air
33      call diel02 (anglei, wavlen, dielec, dielew,
34      &            mipp,iipp, mrpp,rrpp,llpp, ddpp,
35      &            mipa,iipa, mrpa,rrpa,llpa, ddpa)
36      goto 101
37  c -----
38  3 continue      ! Silicon (crystalline)
39      call diel03 (anglei, wavlen, dielec, dielew,
40      &            mipp,iipp, mrpp,rrpp,llpp, ddpp,
41      &            mipa,iipa, mrpa,rrpa,llpa, ddpa)
42      goto 101
43  c -----
44  4 continue      ! Silicon (amorphous)
45      call diel04 (anglei, wavlen, dielec, dielew,
46      &            mipp,iipp, mrpp,rrpp,llpp, ddpp,
47      &            mipa,iipa, mrpa,rrpa,llpa, ddpa)
48      goto 101
49  c -----
50  5 continue      ! Silicon Dioxide (glass)

```

```

51      call diel05 (anglei, wavlen, dielec, dielew,
52      &           mipp,iipp, mrpp,rrpp,llpp, ddpp,
53      &           mipa,iipa, mrpa,rrpa,llpa, ddpa)
54      goto 101
55  c -----
56      6 continue      ! Silicon Nitride (noncrystalline)
57      call diel06 (anglei, wavlen, dielec, dielew,
58      &           mipp,iipp, mrpp,rrpp,llpp, ddpp,
59      &           mipa,iipa, mrpa,rrpa,llpa, ddpa)
60      goto 101
61  c -----
62      7 continue      ! Germanium (crystalline)
63      call diel07 (anglei, wavlen, dielec, dielew,
64      &           mipp,iipp, mrpp,rrpp,llpp, ddpp,
65      &           mipa,iipa, mrpa,rrpa,llpa, ddpa)
66      goto 101
67  c -----
68      8 continue      ! GaAs (crystalline)
69      call diel08 (anglei, wavlen, dielec, dielew,
70      &           mipp,iipp, mrpp,rrpp,llpp, ddpp,
71      &           mipa,iipa, mrpa,rrpa,llpa, ddpa)
72      goto 101
73  c -----
74      9 continue      ! Al(x) Ga(1-x) As
75      call diel09 (anglei, wavlen, dielec, dielew,
76      &           mipp,iipp, mrpp,rrpp,llpp, ddpp,
77      &           mipa,iipa, mrpa,rrpa,llpa, ddpa)
78      goto 101
79  c -----
80      10 continue     ! Oxides of GaAs, Ga(2)O(3), etc.
81      call diel10 (anglei, wavlen, dielec, dielew,
82      &           mipp,iipp, mrpp,rrpp,llpp, ddpp,
83      &           mipa,iipa, mrpa,rrpa,llpa, ddpa)
84      goto 101
85  c -----
86      11 continue     ! Arsenic (amorphous)
87      call diel11 (anglei, wavlen, dielec, dielew,
88      &           mipp,iipp, mrpp,rrpp,llpp, ddpp,
89      &           mipa,iipa, mrpa,rrpa,llpa, ddpa)
90      goto 101
91  c -----
92      12 continue     ! GaP
93      call diel12 (anglei, wavlen, dielec, dielew,
94      &           mipp,iipp, mrpp,rrpp,llpp, ddpp,
95      &           mipa,iipa, mrpa,rrpa,llpa, ddpa)
96      goto 101
97  c -----
98      13 continue     ! GaSb
99      call diel13 (anglei, wavlen, dielec, dielew,
100     &           mipp,iipp, mrpp,rrpp,llpp, ddpp,
101     &           mipa,iipa, mrpa,rrpa,llpa, ddpa)
102     goto 101
103  c -----

```

```

104 14 continue      ! InAs
105      call diel14 (anglei, wavlen, dielec, dielew,
106      &            mipp,iipp, mrpp,rrpp,llpp, ddpp,
107      &            mipa,iipa, mrpa,rrpa,llpa, ddpa)
108      goto 101
109 c -----
110 15 continue      ! InP
111      call diel15 (anglei, wavlen, dielec, dielew,
112      &            mipp,iipp, mrpp,rrpp,llpp, ddpp,
113      &            mipa,iipa, mrpa,rrpa,llpa, ddpa)
114      goto 101
115 c -----
116 16 continue      ! InSb
117      call diel16 (anglei, wavlen, dielec, dielew,
118      &            mipp,iipp, mrpp,rrpp,llpp, ddpp,
119      &            mipa,iipa, mrpa,rrpa,llpa, ddpa)
120      goto 101
121 c -----
122 17 continue      ! AlSb
123      call diel17 (anglei, wavlen, dielec, dielew,
124      &            mipp,iipp, mrpp,rrpp,llpp, ddpp,
125      &            mipa,iipa, mrpa,rrpa,llpa, ddpa)
126      goto 101
127 c -----
128 18 continue      ! Si *1.01, Geist
129      call diel18 (anglei, wavlen, dielec, dielew,
130      &            mipp,iipp, mrpp,rrpp,llpp, ddpp,
131      &            mipa,iipa, mrpa,rrpa,llpa, ddpa)
132      goto 101
133 c -----
134 19 continue      !
135 c*      call diel19 (anglei, wavlen, dielec, dielew,
136 c*      &            mipp,iipp, mrpp,rrpp,llpp, ddpp,
137 c*      &            mipa,iipa, mrpa,rrpa,llpa, ddpa)
138      if (.true.) stop
139      goto 101
140 c -----
141 20 continue      ! GaAs (Sell, Horowitz)
142      call diel20 (anglei, wavlen, dielec, dielew,
143      &            mipp,iipp, mrpp,rrpp,llpp, ddpp,
144      &            mipa,iipa, mrpa,rrpa,llpa, ddpa)
145      goto 101
146 c -----
147 101 continue
148      return
149
150 102 format (' dielmn, ... oops, ', 2i4, 4x, ' lmnt, nlmnts')
151 103 format (' dielmn, ... oops, update argument list of: GOTO')
152      end

```

6.5 Dielectric Functions, Constituent Media

6.5.1 DIEL01.FOR, vacuum

```
1  c      Optical properties of:    vacuum
2
3      subroutine diel01 (anglei, wavlen, dielec, dielew,
4      &                  mipp,iipp, mrpp,rrpp,llpp, ddpp, ! mixture
5      &                  mipa,iipa, mrpa,rrpa,llpa, ddpa) ! ambient
6
7      integer    iipa(1), iipp(1)
8      real       rrpa(1), rrpp(1), anglei, wavlen
9      integer    llpa(1), llpp(1)
10     complex    ddpa(1), ddpp(1), dielec, dielew
11
12     include 'iounit.'
13     include 'defnit.'
14     include 'elmnts.'
15     include 'handyy.'          ! pi,cccc,wavlev
16
17 c*      common / dieo01 / rfrac, dfrac ! not necessary
18
19
20     if (.not.llmnts(1)) then
21         llmnts(1) = .true.
22         write (iout,111)
23     end if
24
25     dielec = cmplx (1.0, 0.0)      ! dielectric function
26     dielew = cmplx (0.0, 0.0)      ! d/d(energy "eV) (dielec)
27
28     return
29 111 format (' lmnt " 1, filename = vacuum')
30     end
```


6.5.2 DIEL02.FOR, air

```

1  c  -----
2  c  Optical properties of:      air
3
4  c  References:      Frank E. Jones,
5  c  1) "Calculation of Compressibility Factor for Air Over Ranges of
6  c      Pressure, Temperature, and Relative Humidity of Interest in
7  c      Flowmeter Calibration",
8  c      NBSIR 83-2652, National Bureau of Standards, March 1983.
9  c  2) "The Refractivity of Air",
10 c      Journal of Research of the National Bureau of Standards,
11 c      Volume 86, Number 1, January-February, 1981, pages 27-32.
12 c  3) "Simplified Equation for Calculating the Refractivity of Air",
13 c      Applied Optics, Volume 19, Number 24, 15 December 1980,
14 c      pages 4129-4130.
15 c  4) "The Air Density Equation and the Transfer of the Mass Unit",
16 c      Journal of Research of the National Bureau of Standards,
17 c      Volume 83, Number 5, September-October, 1978, pages 419-428.
18
19 c  The optical properties of air is dependent upon:
20 c  a)  molecular composition  (CO2, water vapor, ...)
21 c  b)  pressure,
22 c  c)  temperature.
23 c  -----
24
25  subroutine diel02 (anglei, wavlen, dielec, dielew,
26  &                  mipp,iipp, mrpp,rrpp,llpp, ddpp, ! mixture
27  &                  mipa,iipa, mrpa,rpa,llpa, ddpa) ! ambient
28
29  integer  iipa(1), iipp(1)
30  real     rrpa(1), rrpp(1), anglei, wavlen
31  integer  llpa(1), llpp(1)
32  complex  ddpa(1), ddpp(1), dielec, dielew
33
34  include 'iounit.'
35  include 'defnit.'
36  include 'elmnts.'
37  include 'handyy.'          ! pi,cccc,wavlev
38
39  common / dieo02 / rfrac, dfrac ! (n-1), n'
40
41
42  if (.not.llmnts(2)) then
43      llmnts(2) = .true.
44      write (iout,111)
45  end if
46
47  tz = 273.15                ! zero Celsius expressed in Kelvin
48  ts = tz + 15.0             ! standard air
49  tr = tz + 20.0             ! temperature of room (Kelvin)
50

```

```

51      ps = 760.0                      ! standard air ~ one atmosphere
52      pr = 760.0                      ! pressure in room (torr ~ mm Hg)
53
54      xs = 0.0003                     ! standard air
55      xr = 0.00043                   ! carbon dioxide in room
56
57      us = 0.0                        ! standard air ~ dry
58      ur = 0.50                       ! relative humidity (water) in room
59
60      c -----
61      c Enhancement factor (saturation water vapor pressure: air vs. pure phase)
62
63      f = 1.00070 + (3.113E-8 * 101325.0)*(pr/ps)
64      &      +      5.4E-7 * (tr-tz)**2
65      c -----
66      c Saturation water vapor pressure in (pure phase ?)
67
68      es = 1.7526E+11 * exp (-5315.56 /tr)      ! Pascals
69      c -----
70      c Compressibility of air (standard)
71
72      pp = 1.0                        ! pressure in atmospheres
73      ap = -10.864 + pp*(588.26 - pp*2.7106)
74      bp = 0.33297 - pp*(12.585 - pp*2.0659E-2)
75      cp = -2.4925E-3 + pp*(6.3706E-2 - pp*5.5619E-5)
76      tt = ts-tz                      ! temperature in Celsius
77      zs = ap + tt*(bp + tt*cp)
78      zs = zs - us*(35.0 + us*0.5)      ! relative humidity correction
79      zs = 1.0 - zs*1.0E-6
80      c -----
81      c Compressibility of air (room)
82
83      pp = pr/ps                      ! pressure in atmospheres
84      ap = -10.864 + pp*(588.26 - pp*2.7106)
85      bp = 0.33297 - pp*(12.585 - pp*2.0659E-2)
86      cp = -2.4925E-3 + pp*(6.3706E-2 - pp*5.5619E-5)
87      tt = tr-tz                      ! temperature in Celsius
88      zr = ap + tt*(bp + tt*cp)
89      zr = zr - ur*(35.0 + ur*0.5)      ! relative humidity correction
90      zr = 1.0 - zr*1.0E-6
91      c -----
92      c The source of incident light is characterized by
93      c wavlen:      a) -wavelength in units of nano-meters, or
94      c                b) energy in units of electron-volts.
95      c -----
96      if (wavlen .lt. 0.0) then      ! nm, wavelength
97          sigma = -1.0E3/wavlen      ! um**-1
98      else                          ! eV, energy
99          sigma = 1.0E3*wavlen/wavlev ! um**-1
100     end if
101     ss = sigma*sigma                ! inverse (micro-meter) **2
102
103     airs = 8342.13 + 2406030./((130.0-ss) + 15997.0/(38.9-ss))

```

```

104      airs = airs * 1.0E-8 * (pr/ps)*(ts/tr)*(zs/zr)      ! standard air
105      airx = airs * (1.0 + 0.540*(xr-xs))                  ! x C02
106
107      water = ur*f*es* (4.2922E-2 - ss*3.43E-4) *1.0E-8
108      rfrac = airx - water                                  ! n-1
109      refrac = 1.0 + rfrac                                  ! refractive index
110      dielec = cmplx (refrac*refrac, 0.0)                  ! dielectric function
111  c -----
112  c Derivatives with respect to energy (eV).
113
114      airs = 2406030./(((130.0-ss)**2) + 15997.0/((38.9-ss)**2) ! d/d(ss)
115      airs = airs * 1.0E-8 * (pr/ps)*(ts/tr)*(zs/zr)      ! standard air
116      airx = airs * (1.0 + 0.540*(xr-xs))                  ! x C02
117
118      water = ur*f*es* 3.43E-12                            ! d/d(ss)
119      dfrac = airx - water                                  ! d/d(ss)          " (micro-m)**2
120      dfrac = dfrac * sigma*2.0                            ! d/d(sigma)          " (micro-m)
121      dfrac = dfrac / (wavlev*1.0E-3) ! d/d(energy " eV)
122      dielew = cmplx (refrac*dfrac*2.0, 0.0)              ! d/d(energy "eV) (dielec)
123
124  c* write (iout,103) rfrac, dfrac
125
126      return
127
128      103 format (' rfrac = ', 1pe15.5, ' = (n-1) '
129      &          /' dfrac = ',  e15.5, ' = (n-1)'' ' d/d(energy) (n-1) ')
130      111 format (' lmnt " 2, filename = air')
131      end

```

6.5.3 DIEL03.FOR, Si (crystalline)

```

1  c  -----
2  c  Optical properties of:      Silicon (Si),   crystalline.
3  c  -----
4
5      subroutine diel03 (anglei, wavlen, dielec, dielew,
6      &                  mipp,iipp, mrpp,rrpp,llpp, ddpp, ! mixture
7      &                  mipa,iipa, mrpa,rrpa,llpa, ddpa) ! ambient
8
9      integer  iipa(1), iipp(1)
10     real     rrpa(1), rrpp(1), anglei, wavlen
11     integer  llpa(1), llpp(1)
12     complex  ddpa(1), ddpp(1), dielec, dielew
13
14     include 'iounit.'
15     include 'defnit.'
16     include 'elmnts.'
17     include 'handyy.'                      ! pi,cccc,wavlev
18
19     character*64 filnam
20     character*4  string                      ! convenience
21
22  c  Note:      nx = mx+2,                because of:  dudx(1), dudx(mx)
23  c  in order to include the first derivatives at each end point.
24
25     parameter  (nx = 50,                ko = 4)
26     parameter  (nw = nx*(3*ko-2) + ko*ko + ((ko+1)*(ko+2))/2)
27     common / dieooo3 / t(nx+ko), c(nx,2), x1,x2, mx, iptr
28     common / dieooo / xx(nx), id(nx), iw(nx), w(nw), u(4), v(2)
29
30
31     if (llmnts(3)) goto 2
32
33  c  Fetch information on the dielectric function.
34  c  Assume:  1)  no partitions
35  c           2)  discretization of input data is of either form:
36  c               a)  energy (eV),      refractive index,  extinction
37  c               b)  energy (eV),      dielectric function, conductivity
38
39     filnam = 'Si'                          ! silicon crystalline
40     write (iout,111) filnam
41     filnam = subdir//filnam
42     call ljchar (filnam)                    ! left-justify characters
43     open (iscr, file=filnam, status='old',readonly,shared,err=11)
44  c*  write (iout,111) filnam
45
46     1 read (iscr,112,err=12,end=12) string  ! skip header
47  c*  write (iout,113)                      string
48     if (string .ne. '=h==') goto 1
49
50     read (iscr, *) mx                      ! quantity of input data

```

```

51  c*   write (iout,121) mx                               !   within one partition
52       if (mx.lt.3 .or. mx+2.ne.mx) then
53         write (iout,122)
54         stop
55       end if
56
57       k = 0                                               ! index knots
58       do i=1,mx
59         read (isrc,*,err=13,end=13) x, u
60  c*   write (iout,123) x, u
61
62         if (i.ne.1) then                                ! induce ordering
63           if (x .le. xx(k)) then
64             write (iout,124)
65             stop
66           end if
67         end if
68
69         if (i.eq.2) then                                ! usual case for cubic spline fit
70           k = k+1
71           xx(k) = xx(1)                                  ! energy (eV)
72           id(k) = 1                                     ! i-th derivative
73           c(k,1) = (u(3)-c(1,1)) / (x-xx(1))           ! refractive index
74           c(k,2) = (u(4)-c(1,2)) / (x-xx(1))           ! extinction
75         end if
76
77         k = k+1
78         xx(k) = x                                         ! energy (eV)
79         id(k) = 0                                         ! i-th derivative
80         c(k,1) = u(3)                                     ! refractive index
81         c(k,2) = u(4)                                     ! extinction
82
83         if (i.eq.mx) then                                ! usual case for cubic spline fit
84           k = k+1
85           xx(k) = x                                       ! energy (eV)
86           id(k) = 1                                       ! i-th derivative
87           c(k,1) = (u(3)-c(k-2,1)) / (x-xx(k-2))       ! refractive index
88           c(k,2) = (u(4)-c(k-2,2)) / (x-xx(k-2))       ! extinction
89         end if
90
91       end do      ! x,u
92  c  -----
93     x1 = xx(1)
94     x2 = xx(k)
95     mx = k                                               ! quantity of data points
96
97     do i=1,2
98       call bindk (xx,c(1,i),id,mx,ko, t,c(1,i), w,iw,info)
99       if (info.ne.0) then
100        write (iout,131) info, i
101        call exit (2)
102      end if
103    end do

```



```

104 c =====
105 read (iscr,112,err=12,end=12) string ! end of information
106 c* write (iout,113) string
107 if (string .eq. 'h==') then
108     close (iscr)
109 else
110     write (iout,114)
111     stop
112 end if
113
114 llmnts(3) = .true.
115 iptr = 1 ! initialize
116
117 2 if (wavlen .lt. 0.0) then ! nm, wavelength
118     x = -wavlev /wavlen ! eV <--- nm
119 else
120     x = wavlen ! eV, energy
121 end if
122
123 if (x.lt.x1 .or. x.gt.x2) then ! point exterior domain
124     write (iout,132) x1,x2,x
125     stop
126 end if
127
128 do i=1,2
129     u(i) = bvalu (t,c(1,i),mx,ko, 0,x, iptr,w) ! (n+ik)
130     v(i) = bvalu (t,c(1,i),mx,ko, 1,x, iptr,w) ! (n+ik)'
131 end do
132
133 dielec = cmplx (u(1), u(2)) ! (n+ik)
134 dielew = cmplx (v(1), v(2)) ! (n+ik)'
135
136 dielew = dielec*dielew*cmplx (2.0, 0.0) ! e'
137 dielec = dielec*dielec ! e
138
139 return
140 c =====
141
142 11 write (iout,141)
143     stop
144 12 write (iout,142)
145     stop
146 13 write (iout,143)
147     stop
148
149 111 format ( ' lmnt ~ 3, filename = ', a)
150 112 format ( a)
151 113 format ( ' string = ', a)
152 114 format ( ' oops, error in end-of-info header')
153
154 121 format ( ' mx = ', i5)
155 122 format ( ' oops, inconsistency within: mx')
156 123 format ( 1x, i4, 2x, 3f10.4, 10x, '(j,x,u)' )

```



```

157 124 format ( ' oops, ordering violation ')
158
159 131 format ( ' oops, error in B-spline formation '
160      &      / 10x, 'info =', i2
161      &      / 10x, ' i =', i2 , ', ', 5x, '(1~u, 2~du/dx)' )
162 132 format ( ' oops, evaluation point is exterior domain,'
163      &      / '      x1,x2,x ~ ', 3f10.3)
164
165 141 format ( ' oops, error in opening input data file, ')
166 142 format ( ' oops, error in locating header card, ')
167 143 format ( ' oops, error in reading (i,x,u) ')
168
169      end

```

6.5.4 DIEL04.FOR, Si (amorphous)

```

1  c -----
2  c   Optical properties of:      Silicon (Si),      amorphous.
3  c -----
4
5      subroutine diel04 (anglei, wavlen, dielec, dielew,
6      &                  mipp,iipp, mrpp,rrpp,llpp, ddpp, ! mixture
7      &                  mipa,iipa, mrpa,rpa,llpa, ddpa) ! ambient
8
9      integer   iipa(1), iipp(1)
10     real      rrpa(1), rrpp(1), anglei, wavlen
11     integer   llpa(1), llpp(1)
12     complex   ddpa(1), ddpp(1), dielec, dielew
13
14     include 'iounit.'
15     include 'defnit.'
16     include 'elmnts.'
17     include 'handyy.'                      ! pi,cccc,wavlev
18
19     character*64 filnam
20     character*4  string                      ! convenience
21
22     c   Note:      nx = mx+2,                because of:  dux(1), dux(mx)
23     c   in order to include the first derivatives at each end point.
24
25     parameter   (nx = 27,                    ko = 4)
26     parameter   (nw = nx*(3*ko-2) + ko*ko + ((ko+1)*(ko+2))/2)
27     common / dieooo4 / t(nx+ko), c(nx,2), x1,x2, mx, iptr
28     common / dieooo / xx(nx), id(nx), iw(nx), w(nw), u(2), v(2)
29
30
31     if (llmnts(4)) goto 2
32
33     c   Fetch information on the dielectric function.
34     c   Assume:  1)  no partitions
35     c               2)  discretization of input data is of either form:
36     c                   a)  energy (eV),      refractive index,  extinction
37     c                   b)  energy (eV),  dielectric function,  conductivity
38
39     filnam = 'Sia'                          ! silicon amorphous
40     write (iout,111) filnam
41     filnam = subdix//filnam
42     call ljchar (filnam)                      ! left-justify characters
43     open (iscr, file=filnam, status='old',readonly,shared,err=11)
44     c*   write (iout,111) filnam
45
46     1 read (iscr,112,err=12,end=12) string      ! skip header
47     c*   write (iout,113)                      string
48     if (string.ne. 'h==') goto 1
49
50     read (iscr, *) mx                          ! quantity of input data

```

```

51 c*   write (iout,121) mx                                ! within one partition
52     if (mx.lt.3 .or. mx+2.ne.mx) then
53         write (iout,122)
54         stop
55     end if
56
57     k = 0                                                ! index knots
58     do i=1,mx
59         read (iscr,*,err=13,end=13) x, u
60 c*     write (iout,123) x, u
61
62         if (i.ne.1) then                                ! induce ordering
63             if (x .le. xx(k)) then
64                 write (iout,124)
65                 stop
66             end if
67         end if
68
69         if (i.eq.2) then                                ! usual case for cubic spline fit
70             k = k+1
71             xx(k) = xx(1)                                ! energy (eV)
72             id(k) = 1                                    ! i-th derivative
73             c(k,1) = (u(1)-c(1,1)) / (x-xx(1))          ! refractive index
74             c(k,2) = (u(2)-c(1,2)) / (x-xx(1))          ! extinction
75         end if
76
77         k = k+1
78         xx(k) = x                                        ! energy (eV)
79         id(k) = 0                                        ! i-th derivative
80         c(k,1) = u(1)                                    ! refractive index
81         c(k,2) = u(2)                                    ! extinction
82
83         if (i.eq.mx) then                                ! usual case for cubic spline fit
84             k = k+1
85             xx(k) = x                                    ! energy (eV)
86             id(k) = 1                                    ! i-th derivative
87             c(k,1) = (u(1)-c(k-2,1)) / (x-xx(k-2))      ! refractive index
88             c(k,2) = (u(2)-c(k-2,2)) / (x-xx(k-2))      ! extinction
89         end if
90
91     end do        ! x,u
92 c  -----
93     x1 = xx(1)
94     x2 = xx(k)
95     mx = k                                                ! quantity of data points
96
97     do i=1,2
98         call bindk (xx,c(1,i),id,mx,ko, t,c(1,i), w,iw,info)
99         if (info.ne.0) then
100             write (iout,131) info, i
101             call exit (2)
102         end if
103     end do

```

```

104 c =====
105 read (iscr,112,err=12,end=12) string ! end of information
106 c* write (iout,113) string
107 if (string .eq. 'h==') then
108     close (iscr)
109 else
110     write (iout,114)
111     stop
112 end if
113
114 llmnts(4) = .true.
115 iptr = 1 ! initialize
116
117 2 if (wavlen .lt. 0.0) then ! nm, wavelength
118     x = -wavlev / wavlen ! eV <--- nm
119 else
120     x = wavlen ! eV, energy
121 end if
122
123 if (x.lt.x1 .or. x.gt.x2) then ! point exterior domain
124     write (iout,132) x1,x2,x
125     stop
126 end if
127
128 do i=1,2
129     u(i) = bvalu (t,c(1,i),mx,ko, 0,x, iptr,w) ! (n+ik)
130     v(i) = bvalu (t,c(1,i),mx,ko, 1,x, iptr,w) ! (n+ik)'
131 end do
132
133 dielec = cmplx (u(1), u(2)) ! (n+ik)
134 dielew = cmplx (v(1), v(2)) ! (n+ik)'
135
136 dielew = dielec*dielew*cmplx (2.0, 0.0) ! e'
137 dielec = dielec*dielec ! e
138
139 return
140 c =====
141
142 11 write (iout,141)
143 stop
144 12 write (iout,142)
145 stop
146 13 write (iout,143)
147 stop
148
149 111 format ( ' lmnt ~ 4, filename = ', a)
150 112 format ( a)
151 113 format ( ' string = ', a)
152 114 format ( ' oops, error in end-of-info header')
153
154 121 format ( ' mx = ', i5)
155 122 format ( ' oops, inconsistency within: mx')
156 123 format ( 1x, i4, 2x, 3f10.4, 10x, '(j,x,u)' )

```

```

157 124 format ( ' oops, ordering violation ')
158
159 131 format ( ' oops, error in B-spline formation, '
160      &      / 10x, 'info =', i2
161      &      / 10x, ' i =', i2 , ',', 5x, '(1~u, 2~du/dx)' )
162 132 format ( ' oops, evaluation point is exterior domain,'
163      &      / '      x1,x2,x ^ ', 3f10.3)
164
165 141 format ( ' oops, error in opening input data file, ')
166 142 format ( ' oops, error in locating header card, ')
167 143 format ( ' oops, error in reading (i,x,u) ')
168
169      end

```

6.5.5 DIEL05.FOR, SiO₂ (amorphous)

```

1  c -----
2  c Optical properties of: Silicon Dioxide (SiO2), amorphous glass.
3  c -----
4
5      subroutine diel05 (anglei, wavlen, dielec, dielew,
6      &                  mipp,iipp, mrpp,rrpp,llpp, ddpp, ! mixture
7      &                  mipa,iipa, mrpa,rpa,llpa, ddpa) ! ambient
8
9      integer iipa(1), iipp(1)
10     real rrpa(1), rrpp(1), anglei, wavlen
11     integer llpa(1), llpp(1)
12     complex ddpa(1), ddpp(1), dielec, dielew
13
14     include 'iounit.'
15     include 'defnit.'
16     include 'elmnts.'
17     include 'handyy.' ! pi,cccc,wavlev
18
19     character*64 filnam
20     character*4 string ! convenience
21
22     c Note: nx = mx+2, because of: dux(1), dux(mx)
23     c in order to include the first derivatives at each end point.
24
25     parameter (nx = 48, ko = 4)
26     parameter (nw = nx*(3*ko-2) + ko*ko + ((ko+1)*(ko+2))/2)
27     common / dieo05 / t(nx+ko), c(nx,2), x1,x2, mx, iptr
28     common / dieooo / xx(nx), id(nx), iw(nx), w(nw), u(2), v(2)
29
30
31     if (llmnts(5)) goto 2
32
33     c Fetch information on the dielectric function.
34     c Assume: 1) no partitions
35     c          2) discretization of input data is of either form:
36     c              a) energy (eV), refractive index, extinction
37     c              b) energy (eV), dielectric function, conductivity
38
39     filnam = 'Si_02g' ! silicon dioxide (amorphous glass)
40     write (iout,111) filnam
41     filnam = subdrr/filnam
42     call ljchar (filnam) ! left-justify characters
43     open (iscr, file=filnam, status='old',readonly,shared,err=11)
44     c* write (iout,111) filnam
45
46     1 read (iscr,112,err=12,end=12) string ! skip header
47     c* write (iout,113) string
48     if (string.ne. 'h==') goto 1
49
50     read (iscr, *) mx ! quantity of input data

```



```

51  c*   write (iout,121)  mx                                !   within one partition
52       if (mx.lt.3 .or. mx+2.ne.nx) then
53         write (iout,122)
54         stop
55       end if
56
57       k = 0                                                ! index knots
58       do i=1,mx
59         read (iscr,*,err=13,end=13)  x, u
60  c*   write (iout,123)                                x, u
61
62         if (i.ne.1) then                                  ! induce ordering
63           if (x .le. xx(k)) then
64             write (iout,124)
65             stop
66           end if
67         end if
68
69         if (i.eq.2) then                                  ! usual case for cubic spline fit
70           k = k+1
71           xx(k) = xx(1)                                  ! energy (eV)
72           id(k) = 1                                       ! i-th derivative
73           c(k,1) = (u(1)-c(1,1)) / (x-xx(1))             ! refractive index
74           c(k,2) = (u(2)-c(1,2)) / (x-xx(1))             ! extinction
75         end if
76
77         k = k+1
78         xx(k) = x                                         ! energy (eV)
79         id(k) = 0                                         ! i-th derivative
80         c(k,1) = u(1)                                     ! refractive index
81         c(k,2) = u(2)                                     ! extinction
82
83         if (i.eq.mx) then                                  ! usual case for cubic spline fit
84           k = k+1
85           xx(k) = x                                       ! energy (eV)
86           id(k) = 1                                       ! i-th derivative
87           c(k,1) = (u(1)-c(k-2,1)) / (x-xx(k-2))         ! refractive index
88           c(k,2) = (u(2)-c(k-2,2)) / (x-xx(k-2))         ! extinction
89         end if
90
91       end do      ! x,u
92  c  -----
93     x1 = xx(1)
94     x2 = xx(k)
95     mx = k                                               ! quantity of data points
96
97     do i=1,2
98       call bindk (xx,c(1,i),id,mx,ko, t,c(1,i), w,iw,info)
99       if (info.ne.0) then
100        write (iout,131)  info, i
101        call exit (2)
102      end if
103    end do

```

```

104 c      =====
105      read (iscr,112,err=12,end=12) string      ! end of information
106 c*      write (iout,113)                        string
107      if (string .eq. 'h==') then
108          close (iscr)
109      else
110          write (iout,114)
111          stop
112      end if
113
114      llmnts(5) = .true.
115      iptr = 1                                     ! initialize
116
117      2 if (wavlen .lt. 0.0) then                  ! nm, wavelength
118          x = -wavlev / wavlen                    !      eV <--- nm
119      else
120          x = wavlen                              !      eV, energy
121      end if
122
123      if (x.lt.x1 .or. x.gt.x2) then              ! point exterior domain
124          write (iout,132) x1,x2,x
125          stop
126      end if
127
128      do i=1,2
129          u(i) = bvalu (t,c(1,i),mx,ko, 0,x, iptr,w) ! (n+ik)
130          v(i) = bvalu (t,c(1,i),mx,ko, 1,x, iptr,w) ! (n+ik)'
131      end do
132
133      dielec = cmplx (u(1), u(2))                 ! (n+ik)
134      dielew = cmplx (v(1), v(2))                 ! (n+ik)'
135
136      dielew = dielec*dielew*cmplx (2.0, 0.0)     ! e'
137      dielec = dielec*dielec                      ! e
138
139      return
140 c      =====
141
142      11 write (iout,141)
143          stop
144      12 write (iout,142)
145          stop
146      13 write (iout,143)
147          stop
148
149      111 format ( ' lmnt " 5, filename = ', a)
150      112 format ( a)
151      113 format ( ' string = ', a)
152      114 format ( ' oops, error in end-of-info header')
153
154      121 format ( ' mx = ', i5)
155      122 format ( ' oops, inconsistency within:  mx')
156      123 format ( 1x, i4, 2x, 3f10.4, 10x, '(j,x,u)' )

```

```

157 124 format ( ' oops, ordering violation ')
158
159 131 format ( ' oops, error in B-spline formation, '
160      &      / 10x, 'info =', i2
161      &      / 10x, ' i =', i2 , ',', 5x, '(1~u, 2~du/dx)' )
162 132 format ( ' oops, evaluation point is exterior domain,'
163      &      / '      x1,x2,x ~ ', 3f10.3)
164
165 141 format ( ' oops, error in opening input data file, ')
166 142 format ( ' oops, error in locating header card, ')
167 143 format ( ' oops, error in reading (i,x,u) ')
168
169      end

```

6.5.6 DIEL06.FOR, Si₃N₄ (noncrystalline)

```

1  c  -----
2  c  Optical properties of:  Silicon Nitride (Si3N4), non-crystalline.
3  c  -----
4
5      subroutine diel06 (anglei, wavlen, dielec, dielew,
6      &                  mipp,iipp, mrpp,rrpp,llpp, ddpp, ! mixture
7      &                  mipa,iipa, mrpa,rrpa,llpa, ddpa) ! ambient
8
9      integer  iipa(1), iipp(1)
10     real     rrpa(1), rrpp(1), anglei, wavlen
11     integer  llpa(1), llpp(1)
12     complex  ddpa(1), ddpp(1), dielec, dielew
13
14     include 'iounit.'
15     include 'defnit.'
16     include 'elmnts.'
17     include 'handyy.'                ! pi,cccc,wavlev
18
19     character*64 filnam
20     character*4  string                ! convenience
21
22  c  Note:  nx = mx+2,                because of:  dux(1), dux(mx)
23  c  in order to include the first derivatives at each end point.
24
25     parameter  (nx = 21,              ko = 4)
26     parameter  (nw = nx*(3*ko-2) + ko*ko + ((ko+1)*(ko+2))/2)
27     common / die006 / t(nx+ko), c(nx,2), x1,x2, mx, iptr
28     common / die000 / xx(nx), id(nx), iw(nx), w(nw), u(2), v(2)
29
30
31     if (llmnts(6)) goto 2
32
33  c  Fetch information on the dielectric function.
34  c  Assume:  1)  no partitions
35  c           2)  discretization of input data is of either form:
36  c               a)  energy (eV),      refractive index,  extinction
37  c               b)  energy (eV),  dielectric function,  conductivity
38
39     filnam = 'Si3_N4'                ! Silicon Nitride (non-crystalline)
40     write (iout,111) filnam
41     filnam = subdir//filnam
42     call ljchar (filnam)              ! left-justify characters
43     open (iscr, file=filnam, status='old',readonly,shared,err=11)
44  c*  write (iout,111) filnam
45
46     1 read (iscr,112,err=12,end=12) string    ! skip header
47  c*  write (iout,113)                      string
48     if (string .ne. 'h==') goto 1
49
50     read (iscr, *) mx                  ! quantity of input data

```

```

51  c*   write (iout,121) mx                               ! within one partition
52      if (mx.lt.3 .or. mx+2.ne.nx) then
53          write (iout,122)
54          stop
55      end if
56
57      k = 0                                               ! index knots
58      do i=1,mx
59          read (iscr,*,err=13,end=13) x, u
60      c*   write (iout,123)                                x, u
61
62          if (i.ne.1) then                                ! induce ordering
63              if (x .le. xx(k)) then
64                  write (iout,124)
65                  stop
66              end if
67          end if
68
69          u(2) = alog (u(2))                               ! logarithm fit to extinction
70
71          if (i.eq.2) then                                ! usual case for cubic spline fit
72              k = k+1
73              xx(k) = xx(1)                                ! energy (eV)
74              id(k) = 1                                    ! i-th derivative
75              c(k,1) = (u(1)-c(1,1)) / (x-xx(1))          ! refractive index
76              c(k,2) = (u(2)-c(1,2)) / (x-xx(1))          ! extinction
77          end if
78
79          k = k+1
80          xx(k) = x                                         ! energy (eV)
81          id(k) = 0                                         ! i-th derivative
82          c(k,1) = u(1)                                     ! refractive index
83          c(k,2) = u(2)                                     ! extinction
84
85          if (i.eq.mx) then                                ! usual case for cubic spline fit
86              k = k+1
87              xx(k) = x                                     ! energy (eV)
88              id(k) = 1                                    ! i-th derivative
89              c(k,1) = (u(1)-c(k-2,1)) / (x-xx(k-2))      ! refractive index
90              c(k,2) = (u(2)-c(k-2,2)) / (x-xx(k-2))      ! extinction
91          end if
92
93      end do        ! x,u
94  c  -----
95      x1 = xx(1)
96      x2 = xx(k)
97      mx = k                                               ! quantity of data points
98
99      do i=1,2
100         call bindk (xx,c(1,i),id,mx,ko, t,c(1,i), w,iw,info)
101         if (info.ne.0) then
102             write (iout,131) info, i
103             call exit (2)

```

```

104         end if
105     end do
106 c =====
107     read (iscr,112,err=12,end=12) string      ! end of information
108 c*    write (iout,113)                      string
109     if (string .eq. 'h==') then
110         close (iscr)
111     else
112         write (iout,114)
113         stop
114     end if
115
116     llmnts(6) = .true.
117     iptr = 1                                ! initialize
118
119     2 if (wavlen .lt. 0.0) then                ! nm, wavelength
120         x = -wavlev / wavlen                  !      eV <--- nm
121     else
122         x = wavlen                            !      eV, energy
123     end if
124
125     if (x.lt.x1 .or. x.gt.x2) then            ! point exterior domain
126         write (iout,132) x1,x2,x
127         stop
128     end if
129
130     do i=1,2
131         u(i) = bvalu (t,c(1,i),mx,ko, 0,x, iptr,w) ! (n+ik)
132         v(i) = bvalu (t,c(1,i),mx,ko, 1,x, iptr,w) ! (n+ik)'
133     end do
134
135 c     Logarithmic fit to extinction coefficient, k
136     u(2) = exp (u(2))                        ! k = exp (u)
137     v(2) = u(2)*v(2)                         ! k' = k * u'
138
139     dielec = cmplx (u(1), u(2))              ! (n+ik)
140     dielew = cmplx (v(1), v(2))              ! (n+ik)'
141
142     dielew = dielec*dielew*cmplx (2.0, 0.0)  ! e'
143     dielec = dielec*dielec                   ! e
144
145     return
146 c =====
147
148     11 write (iout,141)
149     stop
150     12 write (iout,142)
151     stop
152     13 write (iout,143)
153     stop
154
155     111 format ( ' lmnt " 6, filename = ', a)
156     112 format ( a)

```



```

157 113 format ( ' string = ', a)
158 114 format ( ' oops, error in end-of-info header')
159
160 121 format ( ' mx = ', i5)
161 122 format ( ' oops, inconsistency within: mx')
162 123 format ( 1x, i4, 2x, 3f10.4, 10x, '(j,x,u)' )
163 124 format ( ' oops, ordering violation ')
164
165 131 format ( ' oops, error in B-spline formation '
166      &      / 10x, 'info =', i2
167      &      / 10x, ' i =', i2 , ', ', 5x, '(1~u, 2~du/dx)' )
168 132 format ( ' oops, evaluation point is exterior domain,'
169      &      / '      x1,x2,x ~ ', 3f10.3)
170
171 141 format ( ' oops, error in opening input data file ')
172 142 format ( ' oops, error in locating header card, ')
173 143 format ( ' oops, error in reading (i,x,u) ')
174
175      end

```

6.5.7 DIEL07.FOR, Ge (crystalline)

```

1  c -----
2  c   Optical properties of:      Germanium (Ge),  crystalline.
3  c -----
4
5      subroutine diel07 (anglei, wavlen, dielec, dielew,
6      &                  mipp,iipp, mrpp,rrpp,llpp,  ddpp, ! mixture
7      &                  mipa,iipa, mrpa,rrpa,llpa,  ddpa) ! ambient
8
9      integer   iipa(1), iipp(1)
10     real      rrpa(1), rrpp(1), anglei, wavlen
11     integer   llpa(1), llpp(1)
12     complex   ddpa(1), ddpp(1), dielec, dielew
13
14     include 'iounit.'
15     include 'defnit.'
16     include 'elmnts.'
17     include 'handyy.'                ! pi,cccc,wavlev
18
19     character*64 filnam
20     character*4  string                ! convenience
21
22  c   Note:   nx = mx+2,                because of:   dux(1), dux(mx)
23  c   in order to include the first derivatives at each end point.
24
25     parameter  (nx = 93,                ko = 4)
26     parameter  (nw = nx*(3*ko-2) + ko*ko + ((ko+1)*(ko+2))/2)
27     common / diecoo7 / t(nx+ko), c(nx,2), x1,x2, mx, iptr
28     common / dieooo / xx(nx), id(nx), iw(nx), w(nw), u(2), v(2)
29
30
31     if (llmnts(7)) goto 2
32
33  c   Fetch information on the dielectric function.
34  c   Assume:  1)  no partitions
35  c             2)  discretization of input data is of either form:
36  c                 a)  energy (eV),      refractive index,  extinction
37  c                 b)  energy (eV),      dielectric function, conductivity
38
39     filnam = 'Ge'                      ! Germanium crystalline
40     write (iout,111) filnam
41     filnam = subdix//filnam
42     call ljchar (filnam)                ! left-justify characters
43     open (iscr, file=filnam, status='old',readonly,shared,err=11)
44  c*    write (iout,111) filnam
45
46     1 read  (iscr,112,err=12,end=12) string      ! skip header
47  c*    write (iout,113)                      string
48     if (string .ne. '=h=') goto 1
49
50     read  (iscr, *)  mx                      ! quantity of input data

```

```

51  c*   write (iout,121)  mx                               ! within one partition
52      if (mx.lt.3 .or. mx+2.ne.nx) then
53          write (iout,122)
54          stop
55      end if
56
57      k = 0                                                ! index knots
58      do i=1,mx
59          read (iscr,*,err=13,end=13)  x, u
60  c*   write (iout,123)      x, u
61
62          if (i.ne.1) then                                ! induce ordering
63              if (x .le. xx(k)) then
64                  write (iout,124)
65                  stop
66              end if
67          end if
68
69          if (i.eq.2) then                                ! usual case for cubic spline fit
70              k = k+1
71              xx(k) = xx(1)                                ! energy (eV)
72              id(k) = 1                                    ! i-th derivative
73              c(k,1) = (u(1)-c(1,1)) / (x-xx(1))          ! refractive index
74              c(k,2) = (u(2)-c(1,2)) / (x-xx(1))          ! extinction
75          end if
76
77          k = k+1
78          xx(k) = x                                         ! energy (eV)
79          id(k) = 0                                         ! i-th derivative
80          c(k,1) = u(1)                                     ! refractive index
81          c(k,2) = u(2)                                     ! extinction
82
83          if (i.eq.mx) then                                ! usual case for cubic spline fit
84              k = k+1
85              xx(k) = x                                     ! energy (eV)
86              id(k) = 1                                    ! i-th derivative
87              c(k,1) = (u(1)-c(k-2,1)) / (x-xx(k-2))      ! refractive index
88              c(k,2) = (u(2)-c(k-2,2)) / (x-xx(k-2))      ! extinction
89          end if
90
91      end do      ! x,u
92  c  -----
93      x1 = xx(1)
94      x2 = xx(k)
95      mx = k                                               ! quantity of data points
96
97      do i=1,2
98          call bindk (xx,c(1,i),id,mx,ko, t,c(1,i), w,iw,info)
99          if (info.ne.0) then
100              write (iout,131)  info, i
101              call exit (2)
102          end if
103      end do

```

```

104 c =====
105 read (iscr,112,err=12,end=12) string ! end of information
106 c* write (iout,113) string
107 if (string .eq. 'h==') then
108     close (iscr)
109 else
110     write (iout,114)
111     stop
112 end if
113
114 llmnts(7) = .true.
115 iptr = 1 ! initialize
116
117 2 if (wavlen .lt. 0.0) then ! nm, wavelength
118     x = -wavlev / wavlen ! eV <--- nm
119 else
120     x = wavlen ! eV, energy
121 end if
122
123 if (x.lt.x1 .or. x.gt.x2) then ! point exterior domain
124     write (iout,132) x1,x2,x
125     stop
126 end if
127
128 do i=1,2
129     u(i) = bvalu (t,c(1,i),mx,ko, 0,x, iptr,w) ! (n+ik)
130     v(i) = bvalu (t,c(1,i),mx,ko, 1,x, iptr,w) ! (n+ik)'
131 end do
132
133 dielec = cmplx (u(1), u(2)) ! (n+ik)
134 dielew = cmplx (v(1), v(2)) ! (n+ik)'
135
136 dielew = dielec*dielew*cmplx (2.0, 0.0) ! e'
137 dielec = dielec*dielec ! e
138
139 return
140 c =====
141
142 11 write (iout,141)
143     stop
144 12 write (iout,142)
145     stop
146 13 write (iout,143)
147     stop
148
149 111 format ( ' lmnt " 7, filename = ', a)
150 112 format ( a)
151 113 format ( ' string = ', a)
152 114 format ( ' oops, error in end-of-info header ')
153
154 121 format ( ' mx = ', i5)
155 122 format ( ' oops, inconsistency within: mx')
156 123 format ( 1x, i4, 2x, 3f10.4, 10x, '(j,x,u)' )

```

```

157 124 format ( ' oops, ordering violation ')
158
159 131 format ( ' oops, error in B-spline formation, '
160      &      / 10x, 'info =', i2
161      &      / 10x, ' i =', i2 , ',', 5x, '(1~u, 2~du/dx)' )
162 132 format ( ' oops, evaluation point is exterior domain , '
163      &      / '      x1,x2,x ~ ', 3f10.3)
164
165 141 format ( ' oops, error in opening input data file, ')
166 142 format ( ' oops, error in locating header card, ')
167 143 format ( ' oops, error in reading (i,x,u) ')
168
169      end

```

6.5.8 DIEL08.FOR, GaAs (crystalline)

```

1  c -----
2  c  Optical properties of:  Gallium Arsenide (GaAs),  crystalline.
3  c -----
4
5      subroutine diel08 (anglei, wavlen, dielec, dielew,
6  &          mipp,iipp, mrpp,rrpp,llpp, ddpp, ! mixture
7  &          mipa,iipa, mrpa,rpa,llpa, ddpa) ! ambient
8
9      integer  iipa(1), iipp(1)
10     real     rrpa(1), rrpp(1), anglei, wavlen
11     integer  llpa(1), llpp(1)
12     complex  ddpa(1), ddpp(1), dielec, dielew
13
14     include 'iounit.'
15     include 'defnit.'
16     include 'elmnts.'
17     include 'handyy.'                ! pi,cccc,wavlev
18
19     character*64  filnam
20     character*4   string                ! convenience
21
22  c  Note:  nx = mx+2,                because of:  dwdx(1), dwdx(mx)
23  c  in order to include the first derivatives at each end point.
24
25     parameter  (nx = 153,            ko = 4)
26     parameter  (nw = nx*(3*ko-2) + ko*ko + ((ko+1)*(ko+2))/2)
27     common / die008 / t(nx+ko), c(nx,2), x1,x2, mx, iptr
28     common / die000 / xx(nx), id(nx), iw(nx), w(nw), u(2), v(2)
29
30
31     if (llmnts(8)) goto 2
32
33  c  Fetch information on the dielectric function.
34  c  Assume:  1)  no partitions
35  c           2)  discretization of input data is of either form:
36  c               a)  energy (eV),      refractive index,  extinction
37  c               b)  energy (eV),  dielectric function,  conductivity
38
39     filnam = 'Ga_As'                ! Gallium Arsenide
40     write (iout,111) filnam
41     filnam = subdrr/filnam
42     call ljchar (filnam)            ! left-justify characters
43     open (iscr, file=filnam, status='old',readonly,shared,err=11)
44  c*  write (iout,111) filnam
45
46     1 read (iscr,112,err=12,end=12) string    ! skip header
47  c*  write (iout,113)                      string
48     if (string.ne. 'h==') goto 1
49
50     read (iscr, *)  mx                ! quantity of input data

```



```

51 c*   write (iout,121) mx                                ! within one partition
52     if (mx.lt.3 .or. mx+2.ne.nx) then
53         write (iout,122)
54         stop
55     end if
56
57     k = 0                                                ! index knots
58     do i=1,mx
59         read (iscr,*,err=13,end=13) x, u
60 c*     write (iout,123) x, u
61
62         if (i.ne.1) then                                ! induce ordering
63             if (x .le. xx(k)) then
64                 write (iout,124)
65                 stop
66             end if
67         end if
68
69         if (i.eq.2) then                                ! usual case for cubic spline fit
70             k = k+1
71             xx(k) = xx(1)                                ! energy (eV)
72             id(k) = 1                                    ! i-th derivative
73             c(k,1) = (u(1)-c(1,1)) / (x-xx(1))          ! refractive index
74             c(k,2) = (u(2)-c(1,2)) / (x-xx(1))          ! extinction
75         end if
76
77         k = k+1
78         xx(k) = x                                        ! energy (eV)
79         id(k) = 0                                        ! i-th derivative
80         c(k,1) = u(1)                                    ! refractive index
81         c(k,2) = u(2)                                    ! extinction
82
83         if (i.eq.mx) then                                ! usual case for cubic spline fit
84             k = k+1
85             xx(k) = x                                    ! energy (eV)
86             id(k) = 1                                    ! i-th derivative
87             c(k,1) = (u(1)-c(k-2,1)) / (x-xx(k-2))      ! refractive index
88             c(k,2) = (u(2)-c(k-2,2)) / (x-xx(k-2))      ! extinction
89         end if
90
91     end do      ! x,u
92 c -----
93     x1 = xx(1)
94     x2 = xx(k)
95     mx = k                                             ! quantity of data points
96
97     do i=1,2
98         call bindk (xx,c(1,i),id,mx,ko, t,c(1,i), w,iw,info)
99         if (info.ne.0) then
100             write (iout,131) info, i
101             call exit (2)
102         end if
103     end do

```

```

104 c      =====
105      read (iscr,112,err=12,end=12) string      ! end of information
106 c*      write (iout,113)                        string
107      if (string .eq. 'h==') then
108          close (iscr)
109      else
110          write (iout,114)
111          stop
112      end if
113
114      llmnts(8) = .true.
115      iptr = 1                                     ! initialize
116
117      2 if (wavlen .lt. 0.0) then                   ! nm, wavelength
118          x = -wavlev /wavlen                      !      eV <--- nm
119      else
120          x = wavlen                               !      eV, energy
121      end if
122
123      if (x.lt.x1 .or. x.gt.x2) then              ! point exterior domain
124          write (iout,132) x1,x2,x
125          stop
126      end if
127
128      do i=1,2
129          u(i) = bvalu (t,c(1,i),mx,ko, 0,x, iptr,w) ! (n+ik)
130          v(i) = bvalu (t,c(1,i),mx,ko, 1,x, iptr,w) ! (n+ik)'
131      end do
132
133      dielec = cmplx (u(1), u(2))                  ! (n+ik)
134      dielew = cmplx (v(1), v(2))                  ! (n+ik)'
135
136      dielew = dielec*dielew*cmplx (2.0, 0.0)      ! e'
137      dielec = dielec*dielec                       ! e
138
139      return
140 c      =====
141
142      11 write (iout,141)
143          stop
144      12 write (iout,142)
145          stop
146      13 write (iout,143)
147          stop
148
149      111 format ( ' lmnt " 8, filename = ', a)
150      112 format ( a)
151      113 format ( ' string = ', a4 )
152      114 format ( ' oops, error in end-of-info header')
153
154      121 format ( ' mx = ', i5)
155      122 format ( ' oops, inconsistency within: mx')
156      123 format ( 1x, i4, 2x, 3f10.4, 10x, '(j,x,u)' )

```

```

157 124 format ( ' oops, ordering violation ' )
158
159 131 format ( ' oops, error in B-spline formation, '
160      &      / 10x, 'info =', i2
161      &      / 10x, ' i =', i2 , ',', 5x, '(1~u, 2~du/dx)' )
162 132 format ( ' oops, evaluation point is exterior domain,'
163      &      / '      x1,x2,x ~ ', 3f10.3)
164
165 141 format ( ' oops, error in opening input data file ' )
166 142 format ( ' oops, error in locating header card, ' )
167 143 format ( ' oops, error in reading (i,x,u) ' )
168
169      end

```

6.5.9 DIEL09.FOR, $\text{Al}_x\text{Ga}_{1-x}\text{As}$ (crystalline)

```

1  c  -----
2  c  Optical properties of:      Aluminum Gallium Arsenide
3  c  Al(x)      Ga(1-x) As
4
5  c  Fetch information on the dielectric function.
6  c  Here, we assume that:
7  c  1) partitions involve distinct composition/stoichiometry
8  c  2) each partition has its OWN discretization (energy)
9  c  3) discretization of the input data file is of either form:
10 c      i) energy (eV),      refractive index,  extinction coeff.
11 c      ii) energy (eV), dielectric function,  conductivity
12 c  -----
13
14      subroutine diel09 (anglei, wavlen, dielec, dielew,
15 &                      mipp,iipp, mrpp,rrpp,llpp, ddpp, ! mixture
16 &                      mipa,iipa, mrpa,rrpa,llpa, ddpa) ! ambient
17
18      integer iipa(1), iipp(1)
19      real rrpa(1), rrpp(1), anglei, wavlen
20      integer llpa(1), llpp(1)
21      complex ddpa(1), ddpp(1), dielec, dielew
22
23      include 'iounit.'
24      include 'defnit.'
25      include 'elmnts.'
26      include 'handyy.' ! pi,cccc,wavlev
27
28      character*64 filnam
29      character*4 string ! convenience
30      integer kkpp(nparms)
31      complex dielc(2), dielw(2)
32
33 c  Let: MX be the maximum number of grid points in any profile, u(x).
34 c  If we then add-include the first derivatives at the end points,
35 c  dudx(1) & dudx(mx), we need spline fit: nx=mx+2 grid points.
36
37      parameter (ny = 9) ! number of distinct stoichiometries
38 c  parameter (mx = 47) ! max number of points in any profile
39      parameter (nx = 49, ko = 4)
40      parameter (nw = nx*(3*ko-2) + ko*ko + ((ko+1)*(ko+2))/2)
41
42      common / dieo09 / t(nx+ko,ny), c(nx,2,ny),
43 &                      x1,x2, mx, iptrx(ny), mxsave(ny),
44 &                      yy(ny), y1,y2, my, iptry
45      common / dieooo / xx(nx), id(nx), iw(nx), w(nw), u(4), v(2)
46
47
48      if (llmnts(9)) goto 2 ! info already in arrays
49
50      filnam = 'Al_Ga_As' ! Aluminum Gallium Arsenide

```

```

51      write (iout,111) filnam
52      filnam = subdir//filnam
53      call ljchar (filnam)                ! left-justify characters
54      open (iscr, file=filnam, status='old',readonly,shared,err=11)
55 c    write (iout,111) filnam
56      1 read (iscr,112,err=12,end=12) string ! skip header
57 c    write (iout,113)                    string
58      if (string .ne. 'h==') goto 1
59 c    -----
60
61      read (iscr, *) my                    ! quantity of partitions
62 c    write (iout,121) my                  ! distinct compositions
63      if (my.lt.1 .or. my.ne.ny) then      ! involving Aluminum
64          write (iout,122) my, ny
65          stop
66      end if
67      read (iscr,112) string                ! skip delimiter
68
69      do iy=1,my                            ! scan partitions, stoichiometry
70          read (iscr, *) mx, y, jy          ! quantity of input data
71 c      write (iout,131) mx, y, jy          ! within one partition
72
73          if (mx.lt.3 .or.
74 &      y.lt.0.0 .or. y.gt.1.0 .or. jy.ne.iy) then
75              write (iout,132) mx,y,jy, nx,iy
76              stop
77          end if
78          if (iy.ne.1) then                  ! verify ordering
79              if (y .le. yy(iy-1)) then      ! of monotonically
80                  write (iout,133) iy, y      ! increasing
81                  stop                        ! stoichiometry
82              end if
83          end if
84
85          yy(iy) = y                        ! retain composition ~ Al
86          mxsave(iy) = mx                  ! retain number of points
87          k = 0                             ! index knots
88          do i=1,mx                         ! scan energy (eV)
89              read (iscr,*,err=15,end=15) x, u
90 c          write (iout,134)                x, u
91
92              if (i.ne.1) then                ! verify ordering
93                  if (x .le. xx(k)) then      ! of monotonically
94                      write (iout,135)        ! increasing energy
95                      stop
96                  end if
97              end if
98              if (i.eq.2) then                ! usual cubic spline
99                  k = k+1                    ! update index label
100                 id(k) = 1                   ! i-th derivative
101                 xx(k) = xx(1)               ! energy (eV)
102                 h = x-xx(1)                 ! energy increment
103                 c(k,1,iy) = (u(3)-c(1,1,iy)) /h ! refractive index'

```

```

104          c(k,2,iy) = (u(4)-c(1,2,iy)) /h      ! extinction coeff'
105      end if
106
107          k = k+1                                ! update index label
108          id(k) = 0                              ! i-th derivative
109          xx(k) = x                              ! energy (eV)
110          c(k,1,iy) = u(3)                      ! refractive index
111          c(k,2,iy) = u(4)                      ! extinction coeff
112
113          if (i.eq.mx) then                      ! usual cubic spline
114              k = k+1                            ! update index label
115              id(k) = 1                          ! i-th derivative
116              xx(k) = x                          ! energy (eV)
117              h = x-xx(k-2)                      ! energy increment
118              c(k,1,iy) = (u(3)-c(k-2,1,iy)) /h  ! refractive index'
119              c(k,2,iy) = (u(4)-c(k-2,2,iy)) /h  ! extinction coeff'
120          end if
121      end do                                     ! x,u
122  c  -----
123      x1 = xx(1)                                ! minimum
124      x2 = xx(k)                                ! maximum
125      mx = k                                    ! number of points spline fitted
126      do i=1,2
127          call bindk (xx, c(1,i,iy), id, mx, ko,
128      &              t(1,iy), c(1,i,iy),      w,iw,info)
129          if (info.ne.0) then
130              write (iout,151) info, i, iy
131              stop
132          end if
133      end do
134
135      read (iscr,112) string                    ! skip delimiter
136  end do                                       ! stoichiometry
137  c  -----
138      read (iscr,112,err=13,end=13) string      ! end of info
139  c  write (iout,113)                          string
140      if (string .ne. 'h==') goto 14
141
142      close (iscr)
143      llmnts(9) = .true.                      ! info in arrays
144      do iy=1,my
145          iptrx(iy) = 1                       ! initialize
146      end do
147      iptry = 1
148      y1 = yy( 1)                             ! minimum, convenience
149      y2 = yy(my)                             ! maximum
150  c  =====
151
152      2 if (wavlen .lt. 0.0) then                ! nm, wavelength
153          x = -wavlev /wavlen                   !      eV <--- nm
154      else
155          x = wavlen                            !      eV, energy
156      end if

```



```

157      if (x.lt.x1 .or. x.gt.x2) then ! point exterior domain
158          write (iout,161) x1, x2, x
159          stop
160      end if
161
162  c -----
163      if (mipp.eq.0 .or.
164      &   mrpp.eq.0 ) then ! consistency test
165          write (iout,162)
166          stop
167      end if
168      k = 0
169      do i=1,mipp ! discern pointer parameter
170          if (iipp(i) .eq. 9) then ! naive identification-recognition
171              k = k+1 ! index local parameters
172              kkpp(k) = i
173          end if
174      end do
175      if (k.ne.1 .or. k.gt.mrpp) then ! precaution, verification
176          write (iout,163)
177          stop
178      end if
179
180      i = kkpp(k) ! locate composition index
181      y = rrpp(i) ! specify composition " A1
182
183      if (y.lt.y1 .or. y.gt.y2) then ! point exterior domain
184          write (iout,164) y1, y2, y
185          stop
186      end if
187
188      j = 1 ! need one composition, default
189      iy = iptry
190      if (y .eq. yy(1)) then ! lower boundary
191          iy = 1
192          goto 5
193      else if (y .eq. yy(my)) then ! upper boundary
194          iy = my
195          goto 5
196      end if
197      3 if (y .eq. yy(iy)) goto 5 ! grid point
198      if (y .lt. yy(iy)) then ! grid point is high
199          iy = iy-1
200          goto 3
201      end if
202      4 if (y .gt. yy(iy)) then ! grid point is low
203          iy = iy+1
204          if (y .lt. yy(iy)) then ! success
205              j = 2 ! need two compositions
206          else
207              goto 3
208          end if
209      end if

```

```

210
211      5 iptry = iy                      ! yy(iy-1) < y <= yy(iy)
212
213 c    Necessary to evaluate:    de/dy ~ de/d stoichiometry
214
215      iys = -1                        ! step down
216      if (j.eq.1 .and. iy.eq.1) iys=1      ! step up, lower bdry
217      do jj=1,2
218          if (jj.eq.2) iy=iy+iys          ! step down/up
219
220          mx = mxsave(iy)
221
222          do i=1,2
223              u(i) = bvalu (t(1,iy),c(1,i,iy),mx,ko, 0,x, iptrx(iy),w)
224              v(i) = bvalu (t(1,iy),c(1,i,iy),mx,ko, 1,x, iptrx(iy),w)
225          end do
226
227          dielec = cmplx (u(1), u(2))      ! (n+ik)
228          dielew = cmplx (v(1), v(2))      ! (n+ik)'
229          dielew = dielec*dielew*cmplx (2.0, 0.0) ! e'
230          dielec = dielec*dielec          ! e
231          dielc(jj) = dielec
232          dielw(jj) = dielew
233      end do
234      iy = iy-iys                        ! reset
235      diff = yy(iy) - yy(iy+iys)          ! > 0, usually
236      i = kkpp(k)                        ! locate composition
237      ddpp(i) = (dielc(1)-dielc(2)) /cmplx (diff,0.0) ! de/dy
238
239      if (j.eq.1) then                    ! grid point
240          dielec = dielc(1)
241          dielew = dielw(1)
242      else                                ! interpolate, j=2
243          frac = (y-yy(iy-1)) /diff      ! above
244          dielc(1) = dielc(1)*cmplx (frac, 0.0)
245          dielw(1) = dielw(1)*cmplx (frac, 0.0)
246          frac = (yy(iy)-y) /diff        ! below
247          dielc(2) = dielc(2)*cmplx (frac, 0.0)
248          dielw(2) = dielw(2)*cmplx (frac, 0.0)
249          dielec = dielc(1)+dielc(2)      ! linear interpolation
250          dielew = dielw(1)+dielw(2)      ! between compositions
251      end if
252
253      return
254 c    =====
255
256      11 write (iout,115)                ! opening
257          stop
258      12 write (iout,116)                ! end of header
259          stop
260      13 write (iout,117)                ! end of info
261          stop
262      14 write (iout,118)                ! end of info ~ improper

```

```

283      stop
284      15 write (iout,119)                ! (i,x,u)
285      stop
286
287      111 format ( ' lmt " 9, filename = ', a)
288      112 format ( a)
289      113 format ( ' string: ', a)
290
291      115 format ( ' oops, unable to open:  input data file      ')
292      116 format ( ' oops, unable to find:  delimiter of header  ')
293      117 format ( ' oops, unable to find:  delimiter of End-of-Info')
294      118 format ( ' oops, improper delimiting string:  End-of-Info')
295      119 format ( ' oops, unable to read:  (i,x,u)              ')
296
297      121 format ( ' my = ', i5)
298      122 format ( ' oops, inconsistency,  my = ', i5
299      &          /'                               ny = ', i5)
300
301      131 format ( 1x, i4, 2x, f10.4, 2x, i4, 10x, '(mx, y, iy)')
302      132 format ( ' oops, inconsistency among the values:  mx, y, iy'
303      &          / 7x, i4, 2x, f10.4, 2x, i4
304      &          / 7x, i4,          14x,      i4)
305      133 format ( ' oops, violation in ordering:  y'
306      &          /'          iy = ', i4
307      &          /'          y = ', f10.4)
308      134 format ( 1x, i4, 2x, 3f10.4, 10x, '(j,x,u)' )
309      135 format ( ' oops, violation in ordering:  x')
310
311      151 format ( ' oops, error in construction of the B-splines '
312      &          / 10x, 'info =', i2
313      &          / 10x, ' i =', i2, ',', 4x, '(1~u, 2~du/dx)'
314      &          / 10x, ' iy =', i2, ',', 4x, '(amount of Aluminum)')
315
316      161 format ( ' oops, evaluation point is exterior domain, (DIEL09)'
317      &          /'          (x1, x2, x) ~ ', 3(2x, f10.4))
318      162 format ( ' oops, need to pass some parameter, so as to specify '
319      &          /'          ... the composition of Aluminum')
320      163 format ( ' oops, need a pointer from within:  iipp'
321      &          /'          to discern the parameter in:  rrpp')
322      164 format ( ' oops, evaluation point is exterior domain, (DIEL09)'
323      &          /'          (y1, y2, y) ~ ', 3(2x, f10.4))
324
325      end

```

6.5.10 DIEL10.FOR, Oxides of GaAs

```

1  c -----
2  c Optical properties of: Gallium Arsenide Oxide.
3  c There are several oxide stoichiometries.
4  c These include: Ga(2)O(3), GaAsO(4), As(2)O(3).
5  c The order of preference is from (most to least), respectively.
6  c Reference: D.E. Aspnes, G.P. Schwartz, G.J. Gualtieri,
7  c A.A. Studna, and B. Schwartz,
8  c Journal Electrochemical Society,
9  c Volume 128, Number 3, pp. 590-597, (1981).
10 c -----
11
12 subroutine diel10 (anglei, wavlen, dielec, dielew,
13 & mipp,iipp, mrpp,rrpp,llpp, ddpp, ! mixture
14 & mipa,iipa, mrpa,rrpa,llpa, ddpa) ! ambient
15
16 integer iipa(1), iipp(1)
17 real rrpa(1), rrpp(1), anglei, wavlen
18 integer llpa(1), llpp(1)
19 complex ddpa(1), ddpp(1), dielec, dielew
20
21 include 'iounit.'
22 include 'defnit.'
23 include 'elmnts.'
24 include 'handyy.' ! pi,cccc,wavlev
25
26 character*64 filnam
27
28 real eg(4), eo(4)
29 data eg / 0.075, 5.5, 7.5, 18.0 / ! poles, Note: 5.5
30 data eo / 0.35, 1.62, 5.5, 18.8 /
31 data x1, x2 / 1.5, 4.5 / ! domain
32
33 if (.not.llmnts(10)) then ! info already in arrays
34 llmnts(10) = .true. ! info in arrays
35 filnam = 'Ga_As_Oxide' ! Gallium Arsenide Oxide
36 write (iout,111) filnam
37 end if
38 if (mipp.ne.0 .or. mrpp.ne.0) then ! no parameters necessary
39 write (iout,112)
40 stop
41 end if
42
43 if (wavlen .lt. 0.0) then ! nm, wavelength
44 x = -wavlev / wavlen ! eV <--- nm
45 else
46 x = wavlen ! eV, energy
47 end if
48 if (x.lt.x1 .or. x.gt.x2) then ! point exterior domain
49 write (iout,121) x1, x2, x
50 stop

```

```

51      end if
52
53 c    Evaluate analytic expression for the dielectric function.
54
55      diel = 0.0
56      diew = 0.0
57      do i=1,4
58          top = eg(i)*eo(i)
59          bot = eg(i)**2 - x**2
60          rat = top/bot
61          diel = diel + rat                      ! e
62          diew = diew + rat*(x/bot)*2.0          ! e'
63      end do
64
65      dielec = cmplx (1.0+diel, 0.0)             ! e
66      dielew = cmplx (    diew, 0.0)             ! e'
67
68      return
69
70 111 format ( ' lmnt ~ 10, filename = ', a)
71 112 format ( ' oops, no parameters necessary')
72 121 format ( ' oops, evaluation point is exterior domain, (DIEL10)'
73 &          /'          (x1, x2, x) ~ ', 3(2x, f10.4))
74      end

```

6.5.11 DIEL11.FOR, As (amorphous)

```

1  c -----
2  c Dielectric function of amorphous arsenic.
3  c Reference:
4  c   "Optical Properties of Amorphous Arsenic",
5  c   G.N. Greaves, E.A.Davis, and J.Bordas,
6  c   Philosophical Magazine, Vol 34, No.2, pp. 265-290, 1976.
7  c   Specifically, see page 278.
8  c -----
9  c* subroutine diel11 (dielec, dielew, energy)
10  subroutine diel11 (anglei, wavlen, dielec, dielew,
11  & mipp,iipp, mrpp,rrpp,llpp, ddpp, ! mixture
12  & mipa,iipa, mrpa,rrpa,llpa, ddpa) ! ambient
13
14  integer iipa(1), iipp(1)
15  real rrpa(1), rrpp(1), anglei, wavlen
16  integer llpa(1), llpp(1)
17  complex ddpa(1), ddpp(1), dielec, dielew
18  real energy ! eV
19  complex plasma
20
21  include 'iounit.'
22  include 'defnit.'
23  include 'elmnts.'
24  include 'handyy.' ! pi, cccc, wavlev
25
26  data hbarwo / 3.9 / ! natural freq, interband transition, (eV).
27  data hbarwp / 18.0 / ! plasma freq, (eV).
28  data hbtaui / 5.0 / ! damping, (eV).
29
30  c -----
31  if (.not.llmnts(11)) then
32  llmnts(11) = .true.
33  write (iout,11)
34  end if
35
36  if (wavlen .lt. 0.0) then ! nm, wavelength
37  energy = - wavlev/wavlen ! eV <--- nm
38  else
39  energy = wavlen ! eV
40  end if
41  c -----
42
43  plasma = cmplx (hbarwp**2, 0.0)
44
45  t1 = (hbarwo-energy)*(hbarwo+energy)
46  t2 = energy*hbtaui
47  dielec = cmplx (t1, -t2) ! denominator
48
49  tip = energy*2.0 ! d/d(energy)
50  t2p = hbtaui

```



```

51      dielew = (plasma/dielec)*(cmplx (t1p, t2p) /dielec)
52
53      dielec = cmplx (1.0, 0.0) + plasma/dielec
54      return
55
56 11 format ( ' lmnt ~ 11,      amorphous arsenic')
57      end

```

6.5.12 DIEL12.FOR, GaP

```

1  c -----
2  c  Optical properties of:  Gallium Phosphide (GaP),  crystalline.
3  c -----
4
5      subroutine diel12 (anglei, wavlen, dielec, dielew,
6  &                      mipp,iipp, mrpp,rrpp,llpp, ddpp, ! mixture
7  &                      mipa,iipa, mrpa,rpa,llpa, ddpa) ! ambient
8
9      integer  iipa(1), iipp(1)
10     real     rrpa(1), rrpp(1), anglei, wavlen
11     integer  llpa(1), llpp(1)
12     complex  ddpa(1), ddpp(1), dielec, dielew
13
14     include 'iounit.'
15     include 'defnit.'
16     include 'elmnts.'
17     include 'handyy.'                      ! pi,cccc,wavlev
18
19     character*64  filnam
20     character*4   string                      ! convenience
21
22  c  Note:  nx = mx+2,          because of:  dux(1), dux(mx)
23  c  in order to include the first derivatives at each end point.
24  c  Let:   nx > mx+2.
25
26     parameter  (nx = 158,          ko = 4)
27     parameter  (nw = nx*(3*ko-2) + ko*ko + ((ko+1)*(ko+2))/2)
28     common / dieo12 / t(nx+ko), c(nx,2), x1,x2, mx, iptr
29     common / dieooo / xx(nx), id(nx), iw(nx), w(nw), u(2), v(2)
30
31
32     if (llmnts(12)) goto 2
33
34  c  Fetch information on the dielectric function.
35  c  Assume:  1)  no partitions
36  c           2)  discretization of input data is of either form:
37  c               a)  energy (eV),      refractive index,  extinction
38  c               b)  energy (eV),  dielectric function,  conductivity
39
40     filnam = 'Ga_P'                      ! Gallium Phosphide
41     write (iout,111) filnam
42     filnam = subdirdir//filnam
43     call ljchar (filnam)                  ! left-justify characters
44     open (iscr, file=filnam, status='old',readonly,shared,err=11)
45  c*  write (iout,111) filnam
46
47     1 read  (iscr,112,err=12,end=12) string  ! skip header
48  c*  write (iout,113)                      string
49     if (string .ne. 'h==') goto 1
50

```

```

51      read (iscr, *) mx                                ! quantity of input data
52 c*    write (iout,121) mx                              ! within one partition
53      if (mx.lt.3 .or. mx+2.gt.nx) then
54          write (iout,122)
55          stop
56      end if
57
58      k = 0                                              ! index knots
59      do i=1,mx
60          read (iscr,*,err=13,end=13) x, u
61 c*      write (iout,123) x, u
62
63          if (i.ne.1) then                                ! induce ordering
64              if (x .le. xx(k)) then
65                  write (iout,124)
66                  stop
67              end if
68          end if
69
70          if (i.eq.2) then                                ! usual case for cubic spline fit
71              k = k+1
72              xx(k) = xx(1)                                ! energy (eV)
73              id(k) = 1                                    ! i-th derivative
74              c(k,1) = (u(1)-c(1,1)) / (x-xx(1))          ! refractive index
75              c(k,2) = (u(2)-c(1,2)) / (x-xx(1))          ! extinction
76          end if
77
78          k = k+1
79          xx(k) = x                                        ! energy (eV)
80          id(k) = 0                                        ! i-th derivative
81          c(k,1) = u(1)                                    ! refractive index
82          c(k,2) = u(2)                                    ! extinction
83
84          if (i.eq.mx) then                                ! usual case for cubic spline fit
85              k = k+1
86              xx(k) = x                                    ! energy (eV)
87              id(k) = 1                                    ! i-th derivative
88              c(k,1) = (u(1)-c(k-2,1)) / (x-xx(k-2))      ! refractive index
89              c(k,2) = (u(2)-c(k-2,2)) / (x-xx(k-2))      ! extinction
90          end if
91
92      end do      ! x,u
93 c  -----
94      x1 = xx(1)
95      x2 = xx(k)
96      mx = k                                              ! quantity of data points
97
98      do i=1,2
99          call bindk (xx,c(1,i),id,mx,ko, t,c(1,i), w,iw,info)
100         if (info.ne.0) then
101             write (iout,131) info, i
102             call exit (2)
103         end if

```

```

104      end do
105  c      =====
106      read (iscr,112,err=12,end=12) string      ! end of information
107  c*     write (iout,113)                        string
108      if (string .eq. '=h==') then
109          close (iscr)
110      else
111          write (iout,114)
112          stop
113      end if
114
115      llmnts(12) = .true.
116      iptr = 1                                ! initialize
117
118      2 if (wavlen .lt. 0.0) then                ! nm, wavelength
119          x = -wavlev / wavlen                    !      eV <--- nm
120      else
121          x = wavlen                                !      eV, energy
122      end if
123
124      if (x.lt.x1 .or. x.gt.x2) then            ! point exterior domain
125          write (iout,132) x1,x2,x
126          stop
127      end if
128
129      do i=1,2
130          u(i) = bvalu (t,c(1,i),mx,ko, 0,x, iptr,w)      ! (n+ik)
131          v(i) = bvalu (t,c(1,i),mx,ko, 1,x, iptr,w)      ! (n+ik)'
132      end do
133
134      dielec = cmplx (u(1), u(2))                ! (n+ik)
135      dielew = cmplx (v(1), v(2))                ! (n+ik)'
136
137      dielew = dielec*dielew*cmplx (2.0, 0.0)        ! e'
138      dielec = dielec*dielec                      ! e
139
140      return
141  c      =====
142
143      11 write (iout,141)
144          stop
145      12 write (iout,142)
146          stop
147      13 write (iout,143)
148          stop
149
150      111 format ( ' lmnt " 12, filename = ', a)
151      112 format ( a)
152      113 format ( ' string = ', a)
153      114 format ( ' oops, error in end-of-info header')
154
155      121 format ( ' mx = ', i5)
156      122 format ( ' oops, inconsistency within: mx')

```

```

157 123 format ( 1x, i4, 2x, 3f10.4, 10x, '(j,x,u)' )
158 124 format ( ' oops, ordering violation ' )
159
160 131 format ( ' oops, error in B-spline formation, '
161      &      / 10x, 'info =', i2
162      &      / 10x, ' i =', i2, ',', 5x, '(1~u, 2~du/dx)' )
163 132 format ( ' oops, evaluation point is exterior domain,'
164      &      / '      x1,x2,x ~ ', 3f10.3)
165
166 141 format ( ' oops, error in opening input data file ' )
167 142 format ( ' oops, error in locating header card, ' )
168 143 format ( ' oops, error in reading (i,x,u) ' )
169
170      end

```

6.5.13 DIEL13.FOR, GaSb

```

1  c -----
2  c  Optical properties of:  Gallium Antimonide (GaSb),  crystalline.
3  c -----
4
5      subroutine diel13 (anglei, wavlen, dielec, dielew,
6  &                      mipp,iipp, mrpp,rrpp,llpp, ddpp, ! mixture
7  &                      mipa,iipa, mrpa,rrpa,llpa, ddpa) ! ambient
8
9      integer  iipa(1), iipp(1)
10     real     rrpa(1), rrpp(1), anglei, wavlen
11     integer  llpa(1), llpp(1)
12     complex  ddpa(1), ddpp(1), dielec, dielew
13
14     include 'iounit.'
15     include 'defnit.'
16     include 'elmnts.'
17     include 'handyy.'                      ! pi,cccc,wavlev
18
19     character*64  filnam
20     character*4   string                      ! convenience
21
22  c  Note:  nx = mx+2,          because of:  dux(1), dux(mx)
23  c  in order to include the first derivatives at each end point.
24  c  Let:   nx > mx+2.
25
26     parameter  (nx = 48,          ko = 4)
27     parameter  (nw = nx*(3*ko-2) + ko*ko + ((ko+1)*(ko+2))/2)
28     common / dieo13 / t(nx+ko), c(nx,2), x1,x2, mx, iptr
29     common / dieooo / xx(nx), id(nx), iw(nx), w(nw), u(4), v(2)
30
31
32     if (llmnts(13)) goto 2
33
34  c  Fetch information on the dielectric function.
35  c  Assume:  1)  no partitions
36  c           2)  discretization of input data is of either form:
37  c               a)  energy (eV),      refractive index,  extinction
38  c               b)  energy (eV),  dielectric function,  conductivity
39
40     filnam = 'Ga_Sb'                      ! Gallium Antimonide
41     write (iout,111) filnam
42     filnam = subdix//filnam
43     call ljchar (filnam)                  ! left-justify characters
44     open (iscr, file=filnam, status='old',readonly,shared,err=11)
45  c*  write (iout,111) filnam
46
47     1 read  (iscr,112,err=12,end=12) string      ! skip header
48  c*  write (iout,113)                          string
49     if (string .ne. '=h==') goto 1
50

```



```

51      read (iscr, *) mx                                ! quantity of input data
52 c*    write (iout,121) mx                             ! within one partition
53      if (mx.lt.3 .or. mx+2.gt.nx) then
54          write (iout,122)
55          stop
56      end if
57
58      k = 0                                              ! index knots
59      do i=1,mx
60          read (iscr,*,err=13,end=13) x, u
61 c*      write (iout,123) x, u
62
63          if (i.ne.1) then                                ! induce ordering
64              if (x .le. xx(k)) then
65                  write (iout,124)
66                  stop
67              end if
68          end if
69
70          if (i.eq.2) then                                ! usual case for cubic spline fit
71              k = k+1
72              xx(k) = xx(1)                                ! energy (eV)
73              id(k) = 1                                    ! i-th derivative
74              c(k,1) = (u(3)-c(1,1)) / (x-xx(1))          ! refractive index
75              c(k,2) = (u(4)-c(1,2)) / (x-xx(1))          ! extinction
76          end if
77
78          k = k+1
79          xx(k) = x                                         ! energy (eV)
80          id(k) = 0                                         ! i-th derivative
81          c(k,1) = u(3)                                     ! refractive index
82          c(k,2) = u(4)                                     ! extinction
83
84          if (i.eq.mx) then                                ! usual case for cubic spline fit
85              k = k+1
86              xx(k) = x                                     ! energy (eV)
87              id(k) = 1                                    ! i-th derivative
88              c(k,1) = (u(3)-c(k-2,1)) / (x-xx(k-2))      ! refractive index
89              c(k,2) = (u(4)-c(k-2,2)) / (x-xx(k-2))      ! extinction
90          end if
91
92      end do      ! x,u
93 c  -----
94      x1 = xx(1)
95      x2 = xx(k)
96      mx = k                                              ! quantity of data points
97
98      do i=1,2
99          call bindk (xx,c(1,i),id,mx,ko, t,c(1,i), w,iw,info)
100         if (info.ne.0) then
101             write (iout,131) info, i
102             call exit (2)
103         end if

```

```

104      end do
105  c      =====
106      read (iscr,112,err=12,end=12) string      ! end of information
107  c*     write (iout,113)                        string
108      if (string .eq. 'h==') then
109          close (iscr)
110      else
111          write (iout,114)
112          stop
113      end if
114
115      llmnts(13) = .true.
116      iptr = 1                                ! initialize
117
118      2 if (wavlen .lt. 0.0) then                ! nm, wavelength
119          x = -wavlev / wavlen                    !      eV <--- nm
120      else
121          x = wavlen                               !      eV, energy
122      end if
123
124      if (x.lt.x1 .or. x.gt.x2) then            ! point exterior domain
125          write (iout,132) x1,x2,x
126          stop
127      end if
128
129      do i=1,2
130          u(i) = bvalu (t,c(1,i),mx,ko, 0,x, iptr,w)      ! (n+ik)
131          v(i) = bvalu (t,c(1,i),mx,ko, 1,x, iptr,w)      ! (n+ik)'
132      end do
133
134      dielec = cmplx (u(1), u(2))                ! (n+ik)
135      dielew = cmplx (v(1), v(2))                ! (n+ik)'
136
137      dielew = dielec*dielew*cmplx (2.0, 0.0)        ! e'
138      dielec = dielec*dielec                      ! e
139
140      return
141  c      =====
142
143      11 write (iout,141)
144          stop
145      12 write (iout,142)
146          stop
147      13 write (iout,143)
148          stop
149
150      111 format ( ' lmnt ~13, filename = ', a)
151      112 format ( a)
152      113 format ( ' string = ', a)
153      114 format ( ' oops, error in end-of-info header')
154
155      121 format ( ' mx = ', i5)
156      122 format ( ' oops, inconsistency within:  mx')

```

```

157 123 format ( 1x, i4, 2x, 3f10.4, 10x, '(j,x,u)' )
158 124 format ( ' oops, ordering violation ' )
159
160 131 format ( ' oops, error in B-spline formation, '
161      &      / 10x, 'info =', i2
162      &      / 10x, ' i =', i2, ',', 5x, '(1~u, 2~du/dx)' )
163 132 format ( ' oops, evaluation point is exterior domain,'
164      &      / '      x1,x2,x ~ ', 3f10.3)
165
166 141 format ( ' oops, error in opening input data file ' )
167 142 format ( ' oops, error in locating header card, ' )
168 143 format ( ' oops, error in reading (i,x,u) ' )
169
170      end

```

6.5.14 DIEL14.FOR, InAs

```

1  c  -----
2  c  Optical properties of:   Indium Arsenide   (InAs),  crystalline.
3  c  -----
4
5      subroutine diel14 (anglei, wavlen, dielec, dielew,
6  &          mipp,iipp,  mrpp,rrpp,llpp,  ddpp,  ! mixture
7  &          mipa,iipa,  mrpa,rrpa,llpa,  ddpa) ! ambient
8
9      integer  iipa(1), iipp(1)
10     real     rrpa(1), rrpp(1), anglei, wavlen
11     integer  llpa(1), llpp(1)
12     complex  ddpa(1), ddpp(1), dielec, dielew
13
14     include 'iounit.'
15     include 'defnit.'
16     include 'elmnts.'
17     include 'handyy.'          ! pi,cccc,wavlev
18
19     character*64 filnam
20     character*4  string          ! convenience
21
22  c  Note:   nx = mx+2,           because of:  dux(1), dux(mx)
23  c  in order to include the first derivatives at each end point.
24  c  Let:    nx > mx+2.
25
26     parameter  (nx = 48,           ko = 4)
27     parameter  (nw = nx*(3*ko-2) + ko*ko + ((ko+1)*(ko+2))/2)
28     common / dieo14 / t(nx+ko), c(nx,2), x1,x2, mx, iptr
29     common / dieooo / xx(nx), id(nx), iw(nx), w(nw), u(4), v(2)
30
31
32     if (llmnts(14)) goto 2
33
34  c  Fetch information on the dielectric function.
35  c  Assume:  1)  no partitions
36  c           2)  discretization of input data is of either form:
37  c               a)  energy (eV),      refractive index,  extinction
38  c               b)  energy (eV),  dielectric function,  conductivity
39
40     filnam = 'In_As'          ! Indium Arsenide
41     write (iout,111) filnam
42     filnam = subdir//filnam
43     call ljchar (filnam)      ! left-justify characters
44     open (iscr, file=filnam, status='old',readonly,shared,err=11)
45  c*  write (iout,111) filnam
46
47     1 read (iscr,112,err=12,end=12) string      ! skip header
48  c*  write (iout,113)          string
49     if (string .ne. '=h=') goto 1
50

```

```

51      read (iscr, *) mx                                ! quantity of input data
52  c*   write (iout,121) mx                              ! within one partition
53      if (mx.lt.3 .or. mx+2.gt.nx) then
54          write (iout,122)
55          stop
56      end if
57
58      k = 0                                              ! index knots
59      do i=1,mx
60          read (iscr,*,err=13,end=13) x, u
61  c*   write (iout,123) x, u
62
63          if (i.ne.1) then                                ! induce ordering
64              if (x .le. xx(k)) then
65                  write (iout,124)
66                  stop
67              end if
68          end if
69
70          if (i.eq.2) then                                ! usual case for cubic spline fit
71              k = k+1
72              xx(k) = xx(1)                                ! energy (eV)
73              id(k) = 1                                    ! i-th derivative
74              c(k,1) = (u(3)-c(1,1)) / (x-xx(1))          ! refractive index
75              c(k,2) = (u(4)-c(1,2)) / (x-xx(1))          ! extinction
76          end if
77
78          k = k+1
79          xx(k) = x                                        ! energy (eV)
80          id(k) = 0                                        ! i-th derivative
81          c(k,1) = u(3)                                    ! refractive index
82          c(k,2) = u(4)                                    ! extinction
83
84          if (i.eq.mx) then                                ! usual case for cubic spline fit
85              k = k+1
86              xx(k) = x                                    ! energy (eV)
87              id(k) = 1                                    ! i-th derivative
88              c(k,1) = (u(3)-c(k-2,1)) / (x-xx(k-2))      ! refractive index
89              c(k,2) = (u(4)-c(k-2,2)) / (x-xx(k-2))      ! extinction
90          end if
91
92      end do      ! x,u
93  c  -----
94      x1 = xx(1)
95      x2 = xx(k)
96      mx = k                                              ! quantity of data points
97
98      do i=1,2
99          call bindk (xx,c(1,i),id,mx,ko, t,c(1,i), w,iw,info)
100         if (info.ne.0) then
101             write (iout,131) info, i
102             call exit (2)
103         end if

```

```

104     end do
105 c     =====
106     read (iscr,112,err=12,end=12) string      ! end of information
107 c*    write (iout,113)                        string
108     if (string .eq. 'h==') then
109         close (iscr)
110     else
111         write (iout,114)
112         stop
113     end if
114
115     llmnts(14) = .true.
116     iptr = 1                                ! initialize
117
118     2 if (wavlen .lt. 0.0) then                ! nm, wavelength
119         x = -wavlev / wavlen                  !     eV <--- nm
120     else
121         x = wavlen                            !     eV, energy
122     end if
123
124     if (x.lt.x1 .or. x.gt.x2) then            ! point exterior domain
125         write (iout,132) x1,x2,x
126         stop
127     end if
128
129     do i=1,2
130         u(i) = bvalu (t,c(1,i),mx,ko, 0,x, iptr,w) ! (n+ik)
131         v(i) = bvalu (t,c(1,i),mx,ko, 1,x, iptr,w) ! (n+ik)'
132     end do
133
134     dielec = cmplx (u(1), u(2))                ! (n+ik)
135     dielew = cmplx (v(1), v(2))                ! (n+ik)'
136
137     dielew = dielec*dielew*cmplx (2.0, 0.0)    ! e'
138     dielec = dielec*dielec                     ! e
139
140     return
141 c     =====
142
143     11 write (iout,141)
144     stop
145     12 write (iout,142)
146     stop
147     13 write (iout,143)
148     stop
149
150     111 format ( ' lmnt " 14, filename = ', a)
151     112 format ( a)
152     113 format ( ' string = ', a)
153     114 format ( ' oops, error in end-of-info header')
154
155     121 format ( ' mx = ', i5)
156     122 format ( ' oops, inconsistency within:  mx')

```



```

157 123 format ( 1x, i4, 2x, 3f10.4, 10x, '(j,x,u)' )
158 124 format ( ' oops, ordering violation ' )
159
160 131 format ( ' oops, error in B-spline formation, '
161      &      / 10x, 'info =', i2
162      &      / 10x, ' i =', i2 , ',', 5x, '(1~u, 2~du/dx)' )
163 132 format ( ' oops, evaluation point is exterior domain,'
164      &      / '      x1,x2,x ~ ', 3f10.3)
165
166 141 format ( ' oops, error in opening input data file ' )
167 142 format ( ' oops, error in locating header card, ' )
168 143 format ( ' oops, error in reading (i,x,u) ' )
169
170      end

```

6.5.15 DIEL15.FOR, InP

```

1  c  -----
2  c  Optical properties of:   Indium Phosphide   (InP),   crystalline.
3  c  -----
4
5      subroutine diel15 (anglei, wavlen, dielec, dielew,
6  &          mipp,iipp, mrpp,rrpp,llpp, ddpp, ! mixture
7  &          mipa,iipa, mrpa,rrpa,llpa, ddpa) ! ambient
8
9      integer  iipa(1), iipp(1)
10     real     rrpa(1), rrpp(1), anglei, wavlen
11     integer  llpa(1), llpp(1)
12     complex  ddpa(1), ddpp(1), dielec, dielew
13
14     include 'iounit.'
15     include 'defnit.'
16     include 'elmnts.'
17     include 'handyy.'                      ! pi,cccc,wavlev
18
19     character*64 filnam
20     character*4  string                      ! convenience
21
22  c  Note:   nx = mx+2,           because of:   dux(1), dux(mx)
23  c  in order to include the first derivatives at each end point.
24  c  Let:    nx > mx+2.
25
26     parameter  (nx = 48,           ko = 4)
27     parameter  (nw = nx*(3*ko-2) + ko*ko + ((ko+1)*(ko+2))/2)
28     common / dieo15 / t(nx+ko), c(nx,2), x1,x2, mx, iptr
29     common / dieooo / xx(nx), id(nx), iw(nx), w(nw), u(4), v(2)
30
31
32     if (llmnts(15)) goto 2
33
34  c  Fetch information on the dielectric function.
35  c  Assume:  1)  no partitions
36  c           2)  discretization of input data is of either form:
37  c                a)  energy (eV),      refractive index,  extinction
38  c                b)  energy (eV),  dielectric function,  conductivity
39
40     filnam = 'In_P'                      ! Indium Phosphide
41     write (iout,111) filnam
42     filnam = subdrr/filnam
43     call ljchar (filnam)                  ! left-justify characters
44     open (iscr, file=filnam, status='old',readonly,shared,err=11)
45  c*  write (iout,111) filnam
46
47     1 read  (iscr,112,err=12,end=12) string      ! skip header
48  c*  write (iout,113)                          string
49     if (string.ne. '=h==') goto 1
50

```

```

51      read (iscr, *) mx                                ! quantity of input data
52 c*    write (iout,121) mx                              ! within one partition
53      if (mx.lt.3 .or. mx+2.gt.nx) then
54          write (iout,122)
55          stop
56      end if
57
58      k = 0                                              ! index knots
59      do i=1,mx
60          read (iscr,*,err=13,end=13) x, u
61 c*      write (iout,123) x, u
62
63          if (i.ne.1) then                                ! induce ordering
64              if (x .le. xx(k)) then
65                  write (iout,124)
66                  stop
67              end if
68          end if
69
70          if (i.eq.2) then                                ! usual case for cubic spline fit
71              k = k+1
72              xx(k) = xx(1)                                ! energy (eV)
73              id(k) = 1                                    ! i-th derivative
74              c(k,1) = (u(3)-c(1,1)) / (x-xx(1))          ! refractive index
75              c(k,2) = (u(4)-c(1,2)) / (x-xx(1))          ! extinction
76          end if
77
78          k = k+1
79          xx(k) = x                                        ! energy (eV)
80          id(k) = 0                                        ! i-th derivative
81          c(k,1) = u(3)                                    ! refractive index
82          c(k,2) = u(4)                                    ! extinction
83
84          if (i.eq.mx) then                                ! usual case for cubic spline fit
85              k = k+1
86              xx(k) = x                                    ! energy (eV)
87              id(k) = 1                                    ! i-th derivative
88              c(k,1) = (u(3)-c(k-2,1)) / (x-xx(k-2))      ! refractive index
89              c(k,2) = (u(4)-c(k-2,2)) / (x-xx(k-2))      ! extinction
90          end if
91
92      end do      ! x,u
93 c  -----
94      x1 = xx(1)
95      x2 = xx(k)
96      mx = k                                              ! quantity of data points
97
98      do i=1,2
99          call bindk (xx,c(1,i),id,mx,ko, t,c(1,i), w,iw,info)
100         if (info.ne.0) then
101             write (iout,131) info, i
102             call exit (2)
103         end if

```

```

104     end do
105 c     =====
106     read (iscr,112,err=12,end=12) string      ! end of information
107 c*    write (iout,113)                        string
108     if (string .eq. 'h==') then
109         close (iscr)
110     else
111         write (iout,114)
112         stop
113     end if
114
115     llmnts(15) = .true.
116     iptr = 1                                ! initialize
117
118     2 if (wavlen .lt. 0.0) then                ! nm, wavelength
119         x = -wavlev / wavlen                  !      eV <--- nm
120     else
121         x = wavlen                            !      eV, energy
122     end if
123
124     if (x.lt.x1 .or. x.gt.x2) then            ! point exterior domain
125         write (iout,132) x1,x2,x
126         stop
127     end if
128
129     do i=1,2
130         u(i) = bvalu (t,c(1,i),mx,ko, 0,x, iptr,w) ! (n+ik)
131         v(i) = bvalu (t,c(1,i),mx,ko, 1,x, iptr,w) ! (n+ik)'
132     end do
133
134     dielec = cmplx (u(1), u(2))                ! (n+ik)
135     dielew = cmplx (v(1), v(2))                ! (n+ik)'
136
137     dielew = dielec*dielew*cmplx (2.0, 0.0)    ! e'
138     dielec = dielec*dielec                     ! e
139
140     return
141 c     =====
142
143     11 write (iout,141)
144     stop
145     12 write (iout,142)
146     stop
147     13 write (iout,143)
148     stop
149
150     111 format ( ' lmnt ~ 15, filename = ', a)
151     112 format ( a)
152     113 format ( ' string = ', a)
153     114 format ( ' oops, error in end-of-info header')
154
155     121 format ( ' mx = ', i5)
156     122 format ( ' oops, inconsistency within:  mx')

```

```

157 123 format ( 1x, i4, 2x, 3f10.4, 10x, '(j,x,u)' )
158 124 format ( ' oops, ordering violation ' )
159
160 131 format ( ' oops, error in B-spline formation, '
161 & / 10x, 'info =', i2
162 & / 10x, ' i =', i2 , ',', 5x, '(1~u, 2~du/dx)' )
163 132 format ( ' oops, evaluation point is exterior domain,'
164 & / ' x1,x2,x ~ ', 3f10.3)
165
166 141 format ( ' oops, error in opening input data file ' )
167 142 format ( ' oops, error in locating header card, ' )
168 143 format ( ' oops, error in reading (i,x,u) ' )
169
170 end

```

6.5.16 DIEL16.FOR, InSb

```

1  c -----
2  c Optical properties of: Indium Antimonide (InSb), crystalline.
3  c -----
4
5  subroutine diel16 (anglei, wavlen, dielec, dielew,
6  & mipp,iipp, mrpp,rrpp,llpp, ddpp, ! mixture
7  & mipa,iipa, mrpa,rrpa,llpa, ddpa) ! ambient
8
9  integer iipa(1), iipp(1)
10 real rrpa(1), rrpp(1), anglei, wavlen
11 integer llpa(1), llpp(1)
12 complex ddpa(1), ddpp(1), dielec, dielew
13
14 include 'iounit.'
15 include 'defnit.'
16 include 'elmnts.'
17 include 'handyy.' ! pi,cccc,wavlev
18
19 character*64 filnam
20 character*4 string ! convenience
21
22 c Note: nx = mx+2, because of: dux(1), dux(mx)
23 c in order to include the first derivatives at each end point.
24 c Let: nx > mx+2.
25
26 parameter (nx = 48, ko = 4)
27 parameter (nw = nx*(3*ko-2) + ko*ko + ((ko+1)*(ko+2))/2)
28 common / dieo16 / t(nx+ko), c(nx,2), x1,x2, mx, iptr
29 common / dieooo / xx(nx), id(nx), iw(nx), w(nw), u(4), v(2)
30
31
32 if (llmnts(16)) goto 2
33
34 c Fetch information on the dielectric function.
35 c Assume: 1) no partitions
36 c 2) discretization of input data is of either form:
37 c a) energy (eV), refractive index, extinction
38 c b) energy (eV), dielectric function, conductivity
39
40 filnam = 'In_Sb' ! Indium Antimonide
41 write (iout,111) filnam
42 filnam = subdir//filnam
43 call ljchar (filnam) ! left-justify characters
44 open (iscr, file=filnam, status='old',readonly,shared,err=11)
45 c* write (iout,111) filnam
46
47 1 read (iscr,112,err=12,end=12) string ! skip header
48 c* write (iout,113) string
49 if (string .ne. 'h==') goto 1
50

```



```

51      read (iscr, *) mx                                ! quantity of input data
52 c*    write (iout,121) mx                              ! within one partition
53      if (mx.lt.3 .or. mx+2.gt.nx) then
54          write (iout,122)
55          stop
56      end if
57
58      k = 0                                              ! index knots
59      do i=1,mx
60          read (iscr,*,err=13,end=13) x, u
61 c*      write (iout,123)                                x, u
62
63          if (i.ne.1) then                                ! induce ordering
64              if (x .le. xx(k)) then
65                  write (iout,124)
66                  stop
67              end if
68          end if
69
70          if (i.eq.2) then                                ! usual case for cubic spline fit
71              k = k+1
72              xx(k) = xx(1)                                ! energy (eV)
73              id(k) = 1                                    ! i-th derivative
74              c(k,1) = (u(3)-c(1,1)) / (x-xx(1))          ! refractive index
75              c(k,2) = (u(4)-c(1,2)) / (x-xx(1))          ! extinction
76          end if
77
78          k = k+1
79          xx(k) = x                                        ! energy (eV)
80          id(k) = 0                                        ! i-th derivative
81          c(k,1) = u(3)                                    ! refractive index
82          c(k,2) = u(4)                                    ! extinction
83
84          if (i.eq.mx) then                                ! usual case for cubic spline fit
85              k = k+1
86              xx(k) = x                                    ! energy (eV)
87              id(k) = 1                                    ! i-th derivative
88              c(k,1) = (u(3)-c(k-2,1)) / (x-xx(k-2))      ! refractive index
89              c(k,2) = (u(4)-c(k-2,2)) / (x-xx(k-2))      ! extinction
90          end if
91
92      end do                                              ! x,u
93 c  -----
94      x1 = xx(1)
95      x2 = xx(k)
96      mx = k                                              ! quantity of data points
97
98      do i=1,2
99          call bindk (xx,c(1,i),id,mx,ko, t,c(1,i), w,iw,info)
100         if (info.ne.0) then
101             write (iout,131) info, i
102             call exit (2)
103         end if

```

```

104      end do
105  c      =====
106      read (iscr,112,err=12,end=12) string      ! end of information
107  c*     write (iout,113)                        string
108      if (string .eq. 'h==') then
109          close (iscr)
110      else
111          write (iout,114)
112          stop
113      end if
114
115      llmnts(16) = .true.
116      iptr = 1                                ! initialize
117
118      2 if (wavlen .lt. 0.0) then                ! nm, wavelength
119          x = -wavlev /wavlen                    !      eV <--- nm
120      else
121          x = wavlen                             !      eV, energy
122      end if
123
124      if (x.lt.x1 .or. x.gt.x2) then            ! point exterior domain
125          write (iout,132) x1,x2,x
126          stop
127      end if
128
129      do i=1,2
130          u(i) = bvalu (t,c(1,i),mx,ko, 0,x, iptr,w)      ! (n+ik)
131          v(i) = bvalu (t,c(1,i),mx,ko, 1,x, iptr,w)      ! (n+ik)'
132      end do
133
134      dielec = cmplx (u(1), u(2))                ! (n+ik)
135      dielew = cmplx (v(1), v(2))                ! (n+ik)'
136
137      dielew = dielec*dielew*cmplx (2.0, 0.0)        ! e'
138      dielec = dielec*dielec                      ! e
139
140      return
141  c      =====
142
143      11 write (iout,141)
144      stop
145      12 write (iout,142)
146      stop
147      13 write (iout,143)
148      stop
149
150      111 format ( ' lmnt " 16,  filename = ', a)
151      112 format ( a)
152      113 format ( ' string = ', a)
153      114 format ( ' oops,  error in end-of-info header')
154
155      121 format ( ' mx = ', i5)
156      122 format ( ' oops, inconsistency within:  mx')

```

```

157 123 format ( 1x, i4, 2x, 3f10.4, 10x, '(j,x,u)' )
158 124 format ( ' oops, ordering violation ' )
159
160 131 format ( ' oops, error in B-spline formation, '
161      &      / 10x, 'info =', i2
162      &      / 10x, ' i =', i2, ', ', 5x, '(1`u, 2`du/dx)' )
163 132 format ( ' oops, evaluation point is exterior domain,'
164      &      / '      x1,x2,x ` ', 3f10.3)
165
166 141 format ( ' oops, error in opening input data file ' )
167 142 format ( ' oops, error in locating header card, ' )
168 143 format ( ' oops, error in reading (i,x,u) ' )
169
170      end

```

6.5.17 DIEL17.FOR, AlSb

```

1  c -----
2  c  Optical properties of:  Aluminum Antimonide  (AlSb),  crystalline.
3  c -----
4
5      subroutine diel17 (anglei, wavlen, dielec, dielew,
6  &                      mipp,iipp,  mrpp,rrpp,llpp,  ddpp,  ! mixture
7  &                      mipa,iipa,  mrpa,rrpa,llpa,  ddpa) ! ambient
8
9      integer  iipa(1), iipp(1)
10     real     rrpa(1), rrpp(1), anglei, wavlen
11     integer  llpa(1), llpp(1)
12     complex  ddpa(1), ddpp(1), dielec, dielew
13
14     include 'iounit.'
15     include 'defnit.'
16     include 'elmnts.'
17     include 'handyy.'                      ! pi,cccc,wavlev
18
19     character*64 filnam
20     character*4  string                      ! convenience
21
22  c  Note:  nx = mx+2,          because of:  dudx(1), dudx(mx)
23  c  in order to include the first derivatives at each end point.
24  c  Let:   nx > mx+2.
25
26     parameter  (nx = 47,          ko = 4)
27     parameter  (nw = nx*(3*ko-2) + ko*ko + ((ko+1)*(ko+2))/2)
28     common / dieo17 / t(nx+ko), c(nx,2), x1,x2, mx, iptr
29     common / dieooo / xx(nx), id(nx), iw(nx), w(nw), u(4), v(2)
30
31
32     if (llmnts(17)) goto 2
33
34  c  Fetch information on the dielectric function.
35  c  Assume:  1)  no partitions
36  c           2)  discretization of input data is of either form:
37  c                a)  energy (eV),      refractive index,  extinction
38  c                b)  energy (eV),  dielectric function,  conductivity
39
40     filnam = 'Al_Sb'                      ! Aluminum Antimonide
41     write (iout,111) filnam
42     filnam = subdir//filnam
43     call ljchar (filnam)                  ! left-justify characters
44     open (iscr, file=filnam, status='old',readonly,shared,err=11)
45  c*  write (iout,111) filnam
46
47     1 read  (iscr,112,err=12,end=12) string      ! skip header
48  c*  write (iout,113)                          string
49     if (string .ne. '=h==') goto 1
50

```

```

51      read (iscr, *) mx                                ! quantity of input data
52 c*    write (iout,121) mx                              ! within one partition
53      if (mx.lt.3 .or. mx+2.gt.nx) then
54          write (iout,122)
55          stop
56      end if
57
58      k = 0                                              ! index knots
59      do i=1,mx
60          read (iscr,*,err=13,end=13) x, u
61 c*      write (iout,123)                                x, u
62
63          if (i.ne.1) then                                ! induce ordering
64              if (x .le. xx(k)) then
65                  write (iout,124)
66                  stop
67              end if
68          end if
69
70          if (i.eq.2) then                                ! usual case for cubic spline fit
71              k = k+1
72              xx(k) = xx(1)                                ! energy (eV)
73              id(k) = 1                                    ! i-th derivative
74              c(k,1) = (u(3)-c(1,1)) / (x-xx(1))          ! refractive index
75              c(k,2) = (u(4)-c(1,2)) / (x-xx(1))          ! extinction
76          end if
77
78          k = k+1
79          xx(k) = x                                        ! energy (eV)
80          id(k) = 0                                        ! i-th derivative
81          c(k,1) = u(3)                                    ! refractive index
82          c(k,2) = u(4)                                    ! extinction
83
84          if (i.eq.mx) then                                ! usual case for cubic spline fit
85              k = k+1
86              xx(k) = x                                    ! energy (eV)
87              id(k) = 1                                    ! i-th derivative
88              c(k,1) = (u(3)-c(k-2,1)) / (x-xx(k-2))      ! refractive index
89              c(k,2) = (u(4)-c(k-2,2)) / (x-xx(k-2))      ! extinction
90          end if
91
92      end do      ! x,u
93 c  -----
94      x1 = xx(1)
95      x2 = xx(k)
96      mx = k                                              ! quantity of data points
97
98      do i=1,2
99          call bindk (xx,c(1,i),id,mx,ko, t,c(1,i), w,iw,info)
100         if (info.ne.0) then
101             write (iout,131) info, i
102             call exit (2)
103         end if

```

```

104      end do
105  c      =====
106      read (iscr,112,err=12,end=12) string      ! end of information
107  c*     write (iout,113)                        string
108      if (string .eq. 'h==') then
109          close (iscr)
110      else
111          write (iout,114)
112          stop
113      end if
114
115      llmnts(17) = .true.
116      iptr = 1                                ! initialize
117
118      2 if (wavlen .lt. 0.0) then                ! nm, wavelength
119          x = -wavlev / wavlen                    !      eV <--- nm
120      else
121          x = wavlen                                !      eV, energy
122      end if
123
124      if (x.lt.x1 .or. x.gt.x2) then            ! point exterior domain
125          write (iout,132) x1,x2,x
126          stop
127      end if
128
129      do i=1,2
130          u(i) = bvalu (t,c(1,i),mx,ko, 0,x, iptr,w)      ! (n+ik)
131          v(i) = bvalu (t,c(1,i),mx,ko, 1,x, iptr,w)      ! (n+ik)'
132      end do
133
134      dielec = cmplx (u(1), u(2))                ! (n+ik)
135      dielew = cmplx (v(1), v(2))                ! (n+ik)'
136
137      dielew = dielec*dielew*cmplx (2.0, 0.0)        ! e'
138      dielec = dielec*dielec                      ! e
139
140      return
141  c      =====
142
143      11 write (iout,141)
144          stop
145      12 write (iout,142)
146          stop
147      13 write (iout,143)
148          stop
149
150      111 format ( ' lmnt - 17, filename = ', a)
151      112 format ( a)
152      113 format ( ' string = ', a)
153      114 format ( ' oops, error in end-of-info header')
154
155      121 format ( ' mx = ', i5)
156      122 format ( ' oops, inconsistency within:  mx')

```



```

157 123 format ( 1x, i4, 2x, 3f10.4, 10x, '(j,x,u)' )
158 124 format ( ' oops, ordering violation ' )
159
160 131 format ( ' oops, error in B-spline formation, '
161      &      / 10x, 'info =', i2
162      &      / 10x, ' i =', i2, ',', 5x, '(1`u, 2`du/dx)' )
163 132 format ( ' oops, evaluation point is exterior domain,'
164      &      / '      x1,x2,x ` ', 3f10.3)
165
166 141 format ( ' oops, error in opening input data file ' )
167 142 format ( ' oops, error in locating header card, ' )
168 143 format ( ' oops, error in reading (i,x,u) ' )
169
170      end

```

6.6 Databases

6.6.1 W.SI

1 Optical Properties of Silicon

2

3 D.E. Aspnes & A.A. Studna,

4 Physical Review B, Volume 27, Number 2, 1983, January, 15.

5 Pages: 985-1009.

6

7

8 E(eV), <e1>, <e2>, n, k, R, alpha*1.0E3 (cm**-1)

9

```

10 =h==          ~ indicate end of header information
11 48            ~ quantity of lines of data
12 1.500 13.488 0.038 3.673 0.005 0.327 0.78
13 1.600 13.793 0.057 3.714 0.008 0.331 1.25
14 1.700 14.079 0.078 3.752 0.010 0.335 1.80
15 1.800 14.413 0.099 3.796 0.013 0.340 2.38
16 1.900 14.797 0.126 3.847 0.016 0.345 3.15
17 1.959308 15.0684 0.14646 3.88185 0.019 Aspnes
18 2.000 15.254 0.172 3.906 0.022 0.351 4.47
19 2.100 15.754 0.236 3.969 0.030 0.357 6.32
20 2.200 16.334 0.260 4.042 0.032 0.364 7.17
21 2.27037 16.7912 0.35981 4.09794 0.044 Aspnes
22 2.300 16.994 0.396 4.123 0.048 0.372 11.19
23 2.400 17.761 0.508 4.215 0.060 0.380 14.65
24 2.500 18.661 0.630 4.320 0.073 0.390 18.48
25 2.600 19.724 0.803 4.442 0.090 0.400 23.81
26 2.700 20.987 1.193 4.583 0.130 0.412 35.63
27 2.800 22.565 1.548 4.753 0.163 0.426 46.22
28 2.900 24.574 2.017 4.961 0.203 0.442 59.75
29 3.000 27.197 2.807 5.222 0.269 0.461 81.73
30 3.100 30.874 4.321 5.570 0.387 0.496 121.62
31 3.200 36.355 7.636 6.062 0.630 0.518 204.28
32 3.300 43.264 17.717 6.709 1.320 0.561 441.68
33 3.400 35.224 35.282 6.522 2.705 0.592 932.13
34 3.500 22.394 33.818 5.610 3.014 0.575 1069.19
35 3.600 19.124 31.632 5.296 2.987 0.564 1089.90
36 3.700 17.231 31.527 5.156 3.058 0.563 1146.67
37 3.800 15.531 32.229 5.065 3.182 0.568 1225.46
38 3.900 13.965 33.567 5.016 3.346 0.577 1322.69
39 4.000 12.240 35.939 5.010 3.586 0.591 1454.11
40 4.100 9.364 39.947 5.020 3.979 0.614 1653.60
41 4.200 2.371 45.348 4.888 4.639 0.652 1974.84
42 4.300 -12.404 44.095 4.087 5.395 0.703 2351.38
43 4.400 -18.818 33.350 3.120 5.344 0.726 2383.23
44 4.500 -19.815 24.919 2.452 5.082 0.740 2317.99
45 4.600 -17.931 18.601 1.988 4.678 0.742 2181.15
46 4.700 -15.190 15.094 1.764 4.278 0.728 2038.07
47 4.800 -13.087 13.193 1.658 3.979 0.710 1936.06
48 4.900 -11.507 11.974 1.597 3.749 0.693 1862.11

```

49	5.000	-10.242	11.195	1.570	3.565	0.675	1806.67
50	5.100	-9.291	10.776	1.571	3.429	0.658	1772.70
51	5.200	-8.724	10.655	1.589	3.354	0.646	1767.66
52	5.300	-8.751	10.586	1.579	3.353	0.647	1801.26
53	5.400	-9.168	9.907	1.471	3.366	0.663	1842.63
54	5.500	-9.106	8.846	1.340	3.302	0.673	1840.59
55	5.600	-8.726	7.999	1.247	3.206	0.675	1820.07
56	5.700	-8.325	7.400	1.186	3.120	0.673	1802.31
57	5.800	-7.987	6.898	1.133	3.045	0.672	1789.99
58	5.900	-7.721	6.460	1.083	2.982	0.673	1783.51
59	6.000	-7.443	5.877	1.010	2.909	0.677	1769.27
60	=h=		"	indicate end of information			

6.6.2 W.SIA

1 Optical Properties of Silicon (Amorphous) (a-Si).

2

3 Reference:

4 Handbook of Optical Constants, Edited by: Edward D. Palik,
5 (Academic Press, Inc.; Orlando, 1985),
6 Subpart 2, Section: Silicon (Amorphous) (a-Si),
7 pages: 571-586, compiled by: H. Piller,
8 literature: D.T. Pierce and W.E. Spicer,
9 Physical Review B 5, 3017, (1972).
10

11	-----					
12	E(eV),	n,	k,	n(H),	k(H)	
13	-----					
14	=h==	* indicate end of header information				
15	25	* quantity of lines of data				
16	1.500	3.86	0.0812	4.13	2.00E-4	(xxx?)
17	1.600	3.93	0.136	4.25	2.37E-2	(xxix)
18	1.700	4.01	0.199	4.37		(xxi?)
19	1.800	4.09	0.271	4.49		(xxi?)
20	1.900	4.17	0.363	4.59		(xxi?)
21	2.000	4.23	0.461	4.71	0.217	(xxxx)
22	2.200	4.36	0.690	4.926	0.4	(xxii)
23	2.400	4.46	0.969	5.142	0.6	(xxii)
24	2.500	4.47	1.12	5.25	0.992	(xxxx)
25	2.600	4.49	1.28		0.850	(xxii)
26	2.800	4.47	1.64			(xxii)
27	3.000	4.38	2.02	5.43	2.19	(xxxx)
28	3.200	4.17	2.38			(xxii)
29	3.400	3.90	2.66			(xxii)
30	3.500	3.73	2.79	4.59	3.38	(xxxx)
31	3.600	3.55	2.88			
32	3.800	3.21	3.00			
33	4.000	2.87	3.06	3.36	3.92	(xxxx)
34	4.200	2.56	3.04			(xxii)
35	4.400	2.30	2.99			(xxii)
36	4.600	2.07	2.93			(xxii)
37	4.800	1.86	2.85			(xxii)
38	5.000	1.69	2.76	1.66	3.38	(xxxx)
39	5.500	1.35	2.51	1.23	2.99	(xxxx)
40	6.000	1.11	2.28	0.961	2.65	(xxxx)
41	=h==	* indicate end of information				

6.6.3 W.SI_O2G

1 Optical Properties of Silicon Dioxide (glass,amorphous) (SiO₂-g).

2

3 Reference:

4 Handbook of Optical Constants, Edited by: Edward D. Palik,
5 (Academic Press, Inc.; Orlando, 1985),
6 Subpart 2, Section: Silicon Dioxide (Glass) (SiO₂),
7 pages: 749-763, compiled by: H.R. Phillip.

8

9	-----		
10	E(eV),	n,	k
11	-----		
12	=h==	- indicate end of header information	
13	46	- quantity of lines of data	
14	0.91018	1.44621	0.0
15	1.0985	1.44888	0.0
16	1.1449	1.44941	0.0
17	1.2228	1.45025	0.0
18	1.3863	1.45185	0.0
19	1.4550	1.45248	0.0
20	1.7549	1.45515	0.0
21	1.8566	1.45608	0.0
22	1.8892	1.45637	0.0
23	1.9257	1.45671	0.0
24	1.95930784	1.457018	0.0 Malitson
25	2.1041	1.45841	0.0
26	2.1102	1.45847	0.0
27	2.1411	1.45877	0.0
28	2.1489	1.45885	0.0
29	2.2705	1.46008	0.0
30	2.4379	1.46187	0.0
31	2.5504	1.46313	0.0
32	2.6503	1.46429	0.0
33	2.8448	1.46669	0.0
34	3.0640	1.46961	0.0
35	3.3967	1.47453	0.0
36	3.4340	1.47512	0.0
37	3.5770	1.47746	0.0
38	3.6427	1.47858	0.0
39	3.7105	1.47976	0.0
40	3.7542	1.48053	0.0
41	4.1034	1.48719	0.0
42	4.1784	1.48873	0.0
43	4.2848	1.49099	0.0
44	4.4226	1.49404	0.0
45	4.5040	1.49592	0.0
46	4.5940	1.49805	0.0
47	4.6751	1.50004	0.0
48	4.9939	1.50841	0.0
49	5.1674	1.51338	0.0
50	5.2131	1.51474	0.0

51	5.3858	1.52009	0.0
52	5.4680	1.52276	0.0
53	5.7819	1.53371	0.0
54	5.7976	1.53429	0.0
55	6.0	1.543	0.0
56	6.25	1.554	0.0
57	6.5	1.567	0.0
58	6.75	1.582	0.0
59	7.0	1.600	0.0
60	=h==	" indicate end of information	

6.6.4 W.SI3_N4

1 Optical Properties of Silicon Nitride (non-crystalline) (Si3N4).
 2
 3 Reference:
 4 Handbook of Optical Constants, Edited by: Edward D. Palik,
 5 (Academic Press, Inc.; Orlando, 1985),
 6 Subpart 2, Section: Silicon Nitride (non-crystalline) (Si3N4),
 7 pages: 771-774, compiled by: H.R. Phillip.

8
 9 Note: k should be fitted logarithmically within: die106

10	-----			
11	E(eV),	n,	k	
12	-----			
13	=h==	" indicate end of header information		
14	19	" quantity of lines of data		
15	1.0	1.998	1.0E-10	" 0.0
16	1.5	2.008	1.0E-10	
17	2.0	2.022	1.0E-10	
18	2.5	2.041	1.0E-10	
19	3.0	2.066	1.0E-10	
20	3.5	2.099	1.0E-10	
21	4.0	2.141	1.0E-10	
22	4.25	2.167	1.0E-10	" 0.0
23	4.5	2.198	2.2E-4	
24	4.75	2.234	1.2E-3	
25	5.0	2.278	4.9E-3	
26	5.25	2.331	1.1E-2	
27	5.5	2.393	2.9	
28	5.75	2.464	5.7E-2	
29	6.0	2.541	0.102	
30	6.25	2.620	0.174	
31	6.5	2.682	0.273	
32	6.75	2.724	0.380	
33	7.0	2.752	0.493	
34	=h==	" indicate end of information		

6.6.5 W.GE

```

1
2 Optical Properties of:      Germanium (Ge)
3
4 1)   Handbook of Optical Constants of Solids,
5       edited by   Edward D. Palik,
6       (Academic Press, Inc., Orlando, 1985)
7
8 2)   D.E. Aspnes  &  A.A. Studna,
9       Physical Review B,  Volume 27,  Number 2, 1983, January, 15.
10      Pages:   985-1009.
11
12 -----
13 E(eV),      n,      k,      R,      alpha*1.OE3 (cm**-1)
14 -----
15 =h==              * indicate end of header information
16 91              * quantity of lines of data
17 1.500      4.653      0.298      0.419      45.30
18 1.54       4.684      0.316
19 1.600      4.763      0.345      0.428      55.97
20 1.64       4.816      0.364
21 1.700      4.897      0.401      0.439      69.06
22 1.74       4.961      0.430
23 1.800      5.067      0.500      0.453      91.25
24 1.84       5.152      0.537
25 1.900      5.294      0.638      0.471      122.96
26 1.95       5.5       0.66
27 2.000      5.588      0.933      0.495      189.12
28 2.04       5.708      1.150
29 2.100      5.748      1.634      0.523      347.91
30 2.14       5.554      1.924
31 2.200      5.283      2.049      0.516      456.93
32 2.24       5.198      2.125
33 2.300      5.062      2.318      0.519      540.33
34 2.34       4.883      2.434
35 2.400      4.610      2.455      0.508      597.26
36 2.44       4.482      2.429
37 2.500      4.340      2.384      0.492      604.15
38 2.54       4.267      2.353
39 2.600      4.180      2.309      0.480      608.62
40 2.64       4.133      2.281
41 2.700      4.082      2.240      0.471      613.12
42 2.74       4.058      2.215
43 2.800      4.035      2.181      0.464      619.05
44 2.84       4.030      2.162
45 2.900      4.037      2.140      0.461      629.17
46 2.94       4.052      2.135
47 3.000      4.082      2.145      0.463      652.25
48 3.04       4.107      2.164
49 3.100      4.141      2.215      0.471      696.14
50 3.14       4.153      2.262

```

51	3.200	4.157	2.340	0.481	758.90
52	3.24	4.150	2.392		
53	3.300	4.128	2.469	0.490	825.88
54	3.34	4.106	2.517		
55	3.400	4.070	2.579	0.497	888.81
56	3.44	4.048	2.615		
57	3.500	4.020	2.667	0.502	946.01
58	3.54	4.005	2.702		
59	3.600	3.985	2.759	0.509	1006.86
60	3.64	3.974	2.799		
61	3.700	3.958	2.863	0.517	1073.71
62	3.74	3.949	2.909		
63	3.800	3.936	2.986	0.527	1150.29
64	3.84	3.930	3.043		
65	3.900	3.920	3.137	0.539	1240.23
66	3.94	3.916	3.209		
67	4.000	3.905	3.336	0.556	1352.55
68	4.04	3.896	3.436		
69	4.100	3.869	3.614	0.579	1501.84
70	4.14	3.837	3.756		
71	4.200	3.745	4.009	0.612	1706.55
72	4.24	3.633	4.207		
73	4.300	3.338	4.507	0.659	1964.58
74	4.34	3.038	4.653		
75	4.400	2.516	4.669	0.705	2082.48
76	4.44	2.226	4.543		
77	4.500	1.953	4.297	0.713	1960.14
78	4.54	1.839	4.147		
79	4.600	1.720	3.960	0.702	1846.52
80	4.64	1.659	3.852		
81	4.700	1.586	3.709	0.690	1767.14
82	4.74	1.546	3.624		
83	4.800	1.498	3.509	0.677	1707.30
84	4.84	1.470	3.439		
85	4.900	1.435	3.342	0.664	1659.73
86	4.94	1.417	3.282		
87	5.000	1.394	3.197	0.650	1620.15
88	5.04	1.382	3.146		
89	5.100	1.370	3.073	0.636	1588.72
90	5.14	1.366	3.031		
91	5.200	1.364	2.973	0.622	1567.25
92	5.24	1.366	2.938		
93	5.300	1.371	2.897	0.609	1556.15
94	5.34	1.377	2.877		
95	5.400	1.383	2.854	0.600	1562.04
96	5.44	1.387	2.849		
97	5.500	1.380	2.842	0.598	1584.57
98	5.54	1.372	2.842		
99	5.600	1.360	2.846	0.602	1615.23
100	5.64	1.345	2.852		
101	5.700	1.310	2.866	0.613	1656.06
102	5.74	1.273	2.874		
103	5.800	1.209	2.873	0.632	1689.07

104	5.84	1.167	2.862		
105	5.900	1.108	2.831	0.644	1693.31
106	5.94	1.073	2.801		
107	6.000	1.023	2.774	0.653	1686.84
108	=h==				indicate end of information

6.6.6 W.GA_AS

1	-----				
2	Optical Properties of: Gallium Arsenide (GaAs)				
3					
4	1) Handbook of Optical Constants of Solids,				
5	edited by Edward D. Palik,				
6	(Academic Press, Inc., Orlando, 1985).				
7					
8	2) D.E. Aspnes & A.A. Studna,				
9	Physical Review B, Volume 27, Number 2, 1983 January 15,				
10	Pages: 985-1009.				
11					
12	-----				
13	E(eV),	n,	k,	R,	alpha*1.0E3 (cm**-1)
14	-----				
15	=h==	~ indicate end of header information			
16	151	~ quantity of lines of data			
17	1.500	3.666	0.080	0.327	12.21
18	1.52	3.672	0.083		
19	1.54	3.679	0.085		
20	1.56	3.685	0.087		
21	1.58	3.693	0.089		
22	1.600	3.700	0.091	0.330	14.83
23	1.62	3.707	0.093		
24	1.64	3.716	0.097		
25	1.66	3.725	0.101		
26	1.68	3.734	0.105		
27	1.700	3.742	0.112	0.335	19.28
28	1.72	3.752	0.118		
29	1.74	3.762	0.127		
30	1.76	3.772	0.134		
31	1.78	3.779	0.152		
32	1.800	3.785	0.151	0.339	27.49
33	1.82	3.792	0.158		
34	1.84	3.799	0.168		
35	1.86	3.809	0.173		
36	1.88	3.817	0.173		
37	1.900	3.826	0.179	0.344	34.45
38	1.92	3.836	0.183		
39	1.94	3.846	0.187		
40	1.96	3.856	0.196		
41	1.98	3.867	0.203		
42	2.000	3.878	0.211	0.349	42.79
43	2.02	3.890	0.213		
44	2.04	3.902	0.223		
45	2.06	3.914	0.228		
46	2.08	3.927	0.232		
47	2.100	3.940	0.240	0.356	51.15
48	2.12	3.954	0.245		
49	2.14	3.968	0.251		
50	2.16	3.983	0.257		

51	2.18	3.998	0.266		
52	2.200	4.013	0.276	0.363	61.46
53	2.22	4.029	0.285		
54	2.24	4.045	0.294		
55	2.26	4.063	0.301		
56	2.28	4.082	0.308		
57	2.300	4.100	0.320	0.372	74.56
58	2.32	4.120	0.327		
59	2.34	4.141	0.337		
60	2.36	4.162	0.347		
61	2.38	4.183	0.359		
62	2.400	4.205	0.371	0.382	90.34
63	2.42	4.229	0.385		
64	2.44	4.254	0.398		
65	2.46	4.279	0.411		
66	2.48	4.305	0.426		
67	2.500	4.333	0.441	0.395	111.74
68	2.52	4.362	0.458		
69	2.54	4.392	0.476		
70	2.56	4.423	0.497		
71	2.58	4.456	0.517		
72	2.600	4.492	0.539	0.410	142.02
73	2.62	4.525	0.569		
74	2.64	4.567	0.595		
75	2.66	4.605	0.626		
76	2.68	4.649	0.659		
77	2.700	4.694	0.696	0.429	190.53
78	2.72	4.741	0.739		
79	2.74	4.793	0.789		
80	2.76	4.845	0.846		
81	2.78	4.902	0.912		
82	2.800	4.959	0.991	0.456	281.33
83	2.82	5.015	1.088		
84	2.84	5.065	1.206		
85	2.86	5.102	1.353		
86	2.88	5.107	1.529		
87	2.900	5.052	1.721	0.490	505.75
88	2.92	4.917	1.885		
89	2.94	4.755	1.960		
90	2.96	4.626	1.967		
91	2.98	4.550	1.952		
92	3.000	4.509	1.948	0.472	592.48
93	3.02	4.483	1.961		
94	3.04	4.462	1.988		
95	3.06	4.439	2.029		
96	3.08	4.413	2.082		
97	3.100	4.373	2.146	0.477	674.17
98	3.12	4.313	2.212		
99	3.14	4.229	2.270		
100	3.16	4.126	2.304		
101	3.18	4.023	2.307		
102	3.200	3.938	2.288	0.468	742.21
103	3.22	3.871	2.260		

104	3.24	3.818	2.232		
105	3.26	3.776	2.207		
106	3.28	3.740	2.183		
107	3.300	3.709	2.162	0.447	723.09
108	3.32	3.681	2.142		
109	3.34	3.657	2.123		
110	3.36	3.635	2.107		
111	3.38	3.614	2.091		
112	3.400	3.596	2.076	0.434	715.28
113	3.42	3.580	2.062		
114	3.44	3.566	2.049		
115	3.46	3.553	2.036		
116	3.48	3.541	2.024		
117	3.500	3.531	2.013	0.425	714.20
118	3.54	3.513	1.992		
119	3.600	3.495	1.965	0.419	717.14
120	3.64	3.489	1.950		
121	3.700	3.485	1.931	0.415	724.14
122	3.74	3.488	1.920		
123	3.800	3.501	1.909	0.414	735.28
124	3.84	3.512	1.905		
125	3.900	3.538	1.904	0.416	752.62
126	3.94	3.559	1.907		
127	4.000	3.601	1.920	0.421	778.65
128	4.04	3.634	1.935		
129	4.100	3.692	1.969	0.430	818.23
130	4.14	3.736	2.001		
131	4.200	3.810	2.069	0.444	880.86
132	4.24	3.864	2.132		
133	4.300	3.939	2.260	0.466	984.86
134	4.34	3.981	2.368		
135	4.400	4.015	2.563	0.494	1143.26
136	4.44	4.004	2.715		
137	4.500	3.913	2.919	0.521	1331.28
138	4.54	3.850	3.018		
139	4.600	3.769	3.169	0.540	1477.66
140	4.64	3.708	3.280		
141	4.700	3.598	3.452	0.565	1644.29
142	4.74	3.511	3.574		
143	4.800	3.342	3.770	0.596	1834.18
144	4.84	3.187	3.898		
145	4.900	2.890	4.047	0.633	2009.92
146	4.94	2.654	4.106		
147	5.000	2.273	4.084	0.668	2069.81
148	5.04	2.044	3.992		
149	5.100	1.802	3.795	0.676	1961.86
150	5.14	1.699	3.660		
151	5.200	1.599	3.484	0.661	1836.14
152	5.24	1.552	3.384		
153	5.300	1.499	3.255	0.644	1748.74
154	5.34	1.468	3.181		
155	5.400	1.430	3.079	0.628	1685.29
156	5.44	1.410	3.019		

157	5.500	1.383	2.936	0.613	1636.68
158	5.54	1.367	2.885		
159	5.600	1.349	2.815	0.599	1597.99
160	5.64	1.339	2.772		
161	5.700	1.325	2.710	0.584	1565.73
162	5.74	1.321	2.673		
163	5.800	1.311	2.625	0.571	1543.07
164	5.84	1.304	2.592		
165	5.900	1.288	2.556	0.562	1528.86
166	5.94	1.287	2.523		
167	6.000	1.284	2.472	0.550	1503.20
168	=h==	" indicate end of information			

6.6.7 W.AL_GA_AS

1 Optical Properties of: Aluminium Gallium Arsenide,

2 Al(x) Ga(1-x) As,

3 where: $0 < x < .8$

4

5 D.E.Aspnes, S.M.Kelso, R.A.Logan, R.Bhat,

6 Journal Applied Physics, Volume 60, Number 2, 1986-January-15,

7 Pages: 754-767.

8

9 E(eV), <e1>, <e2>, n, k, R, alpha*1.0E-3 (cm**-1)

10

11 =h== " indicate end of header information

12 9 " quantity of distinct compositions

13 " quantity of lines, composition of Aluminum

14 (mx, y, iy)

15	46	0.0	1				
16	1.500	13.435	0.436	3.666	0.059	0.327	9.03
17	1.600	13.683	0.687	3.700	0.093	0.330	15.06
18	1.700	13.991	0.922	3.742	0.123	0.335	21.22
19	1.800	14.307	1.192	3.786	0.157	0.340	28.72
20	1.900	14.607	1.367	3.826	0.179	0.344	34.40
21	2.000	14.991	1.637	3.878	0.211	0.349	42.79
22	2.100	15.463	1.893	3.940	0.240	0.356	51.15
23	2.200	16.031	2.212	4.013	0.276	0.363	61.46
24	2.300	16.709	2.622	4.100	0.320	0.372	74.56
25	2.400	17.547	3.123	4.205	0.371	0.382	90.34
26	2.500	18.579	3.821	4.333	0.441	0.395	111.74
27	2.600	19.885	4.841	4.492	0.539	0.410	142.02
28	2.700	21.550	6.536	4.694	0.696	0.429	190.53
29	2.800	23.605	9.830	4.959	0.991	0.456	281.33
30	2.900	22.558	17.383	5.052	1.721	0.490	505.75
31	3.000	16.536	17.571	4.509	1.948	0.472	592.48
32	3.100	14.519	18.765	4.373	2.146	0.477	674.17
33	3.200	10.271	18.022	3.938	2.288	0.468	742.21
34	3.300	9.086	16.037	3.709	2.162	0.447	723.09
35	3.400	8.626	14.929	3.596	2.076	0.434	715.28
36	3.500	8.413	14.216	3.531	2.013	0.425	714.20
37	3.600	8.355	13.739	3.495	1.965	0.419	717.14
38	3.700	8.419	13.459	3.485	1.931	0.415	724.14
39	3.800	8.611	13.365	3.501	1.909	0.414	735.28
40	3.900	8.890	13.470	3.538	1.904	0.416	752.62
41	4.000	9.279	13.832	3.601	1.920	0.421	778.65
42	4.100	9.754	14.538	3.692	1.969	0.430	818.23
43	4.200	10.235	15.767	3.810	2.069	0.444	880.86
44	4.300	10.412	17.803	3.939	2.260	0.466	984.86
45	4.400	9.545	20.582	4.015	2.563	0.494	1143.26
46	4.500	6.797	22.845	3.913	2.919	0.521	1331.28
47	4.600	4.163	23.891	3.769	3.169	0.540	1477.66
48	4.700	1.030	24.835	3.598	3.452	0.565	1644.29
49	4.800	-3.045	25.196	3.342	3.770	0.596	1834.17
50	4.900	-8.022	23.394	2.890	4.047	0.633	2009.91
51	5.000	-11.514	18.564	2.273	4.084	0.668	2069.81

51	5.100	-11.156	13.677	1.802	3.795	0.676	1961.86
52	5.200	-9.578	11.143	1.599	3.484	0.661	1836.15
53	5.300	-8.350	9.758	1.499	3.255	0.644	1748.74
54	5.400	-7.435	8.806	1.430	3.079	0.628	1685.29
55	5.500	-6.705	8.123	1.383	2.936	0.613	1636.68
56	5.600	-6.107	7.593	1.349	2.815	0.599	1597.99
57	5.700	-5.589	7.182	1.325	2.710	0.584	1565.73
58	5.800	-5.171	6.882	1.311	2.625	0.571	1543.08
59	5.900	-4.876	6.587	1.288	2.557	0.562	1528.86
60	6.000	-4.511	6.250	1.264	2.472	0.550	1503.21
61	-----						
62	46	0.099	2	(mx, y, iy)			
63	1.500	12.758	0.000	3.572	0.000	0.316	0.00
64	1.600	13.401	0.434	3.661	0.059	0.326	9.62
65	1.700	13.521	0.600	3.678	0.082	0.328	14.06
66	1.800	13.798	0.738	3.716	0.099	0.332	18.13
67	1.900	14.237	0.962	3.775	0.127	0.338	24.54
68	2.000	14.563	1.305	3.820	0.171	0.343	34.63
69	2.100	14.981	1.540	3.876	0.199	0.349	42.29
70	2.200	15.471	1.864	3.940	0.237	0.356	52.74
71	2.300	16.067	2.216	4.018	0.276	0.364	64.29
72	2.400	16.796	2.627	4.111	0.320	0.373	77.73
73	2.500	17.662	3.225	4.220	0.382	0.384	96.83
74	2.600	18.732	4.023	4.353	0.462	0.397	121.79
75	2.700	20.080	5.196	4.518	0.575	0.413	157.38
76	2.800	21.744	7.213	4.725	0.763	0.433	216.63
77	2.900	23.411	11.184	4.968	1.126	0.461	330.89
78	3.000	20.038	17.765	4.838	1.836	0.483	558.25
79	3.100	16.095	17.384	4.460	1.949	0.469	612.35
80	3.200	13.306	18.598	4.253	2.187	0.475	709.22
81	3.300	10.072	17.026	3.864	2.203	0.458	737.04
82	3.400	9.205	15.494	3.690	2.100	0.441	723.61
83	3.500	8.846	14.619	3.601	2.030	0.430	720.13
84	3.600	8.699	14.060	3.552	1.979	0.423	722.19
85	3.700	8.690	13.736	3.532	1.945	0.419	729.33
86	3.800	8.809	13.609	3.537	1.924	0.417	740.99
87	3.900	9.028	13.692	3.566	1.920	0.419	758.97
88	4.000	9.342	14.017	3.618	1.937	0.423	785.31
89	4.100	9.734	14.664	3.697	1.983	0.431	824.19
90	4.200	10.146	15.766	3.801	2.074	0.444	882.91
91	4.300	10.364	17.571	3.922	2.240	0.464	976.34
92	4.400	9.851	20.145	4.017	2.507	0.489	1118.25
93	4.500	7.811	23.065	4.010	2.876	0.519	1311.72
94	4.600	4.236	24.731	3.829	3.229	0.546	1505.64
95	4.700	0.537	25.535	3.611	3.536	0.572	1684.43
96	4.800	-4.119	25.136	3.267	3.846	0.604	1871.41
97	4.900	-8.604	22.369	2.772	4.036	0.637	2004.32
98	5.000	-10.991	17.583	2.207	3.983	0.662	2018.51
99	5.100	-10.408	13.478	1.819	3.704	0.664	1914.68
100	5.200	-9.116	11.220	1.634	3.433	0.651	1809.48
101	5.300	-8.043	9.870	1.531	3.223	0.635	1731.43
102	5.400	-7.227	8.928	1.459	3.059	0.621	1674.24
103	5.500	-6.550	8.225	1.408	2.921	0.607	1628.38

104	5.600	-5.963	7.677	1.371	2.800	0.593	1589.56
105	5.700	-5.468	7.256	1.345	2.698	0.579	1558.54
106	5.800	-5.032	6.937	1.330	2.608	0.565	1533.15
107	5.900	-4.702	6.692	1.318	2.538	0.554	1517.71
108	6.000	-4.321	6.442	1.311	2.457	0.539	1494.49
109	-----						
110	47	0.198	3	(mx, y, iy)			.
111	1.500	11.950	0.000	3.457	0.000	0.304	0.00
112	1.600	12.502	0.017	3.536	0.002	0.313	0.39
113	1.700	13.213	0.013	3.635	0.002	0.323	0.30
114	1.719	13.423	0.02	3.664	0.003		
115	1.800	13.423	0.601	3.662	0.082	0.326	14.97
116	1.900	13.682	0.696	3.700	0.094	0.330	18.11
117	2.000	14.119	0.887	3.759	0.118	0.337	23.92
118	2.100	14.529	1.260	3.815	0.165	0.343	35.16
119	2.200	14.946	1.567	3.871	0.202	0.349	45.13
120	2.300	15.464	1.909	3.940	0.242	0.356	56.49
121	2.400	16.096	2.313	4.022	0.288	0.364	69.94
122	2.500	16.845	2.812	4.118	0.341	0.374	86.51
123	2.600	17.767	3.460	4.235	0.409	0.386	107.66
124	2.700	18.893	4.363	4.375	0.499	0.399	136.45
125	2.800	20.272	5.787	4.547	0.636	0.417	180.59
126	2.900	21.877	8.225	4.757	0.865	0.439	254.16
127	3.000	22.682	13.063	4.943	1.322	0.467	401.85
128	3.100	17.781	17.110	4.607	1.857	0.472	583.43
129	3.200	15.264	17.325	4.379	1.978	0.467	641.61
130	3.300	11.927	17.808	4.084	2.180	0.466	729.24
131	3.400	9.908	16.040	3.792	2.115	0.447	728.85
132	3.500	9.315	14.923	3.668	2.034	0.434	721.70
133	3.600	9.061	14.254	3.602	1.979	0.426	721.98
134	3.700	8.987	13.874	3.572	1.942	0.421	728.35
135	3.800	9.035	13.714	3.568	1.922	0.419	740.28
136	3.900	9.199	13.758	3.588	1.917	0.420	757.87
137	4.000	9.458	14.047	3.633	1.933	0.423	783.89
138	4.100	9.795	14.630	3.701	1.976	0.431	821.32
139	4.200	10.163	15.627	3.795	2.059	0.443	876.48
140	4.300	10.429	17.254	3.911	2.206	0.460	961.42
141	4.400	10.147	19.686	4.018	2.449	0.485	1092.43
142	4.500	8.568	22.715	4.053	2.803	0.514	1278.33
143	4.600	5.008	25.295	3.924	3.223	0.547	1502.86
144	4.700	0.459	26.010	3.638	3.575	0.576	1702.90
145	4.800	-4.468	25.047	3.238	3.867	0.607	1881.50
146	4.900	-8.500	21.861	2.734	3.997	0.634	1985.28
147	5.000	-10.433	17.302	2.210	3.914	0.655	1983.56
148	5.100	-9.895	13.595	1.860	3.654	0.654	1889.12
149	5.200	-8.795	11.429	1.677	3.407	0.643	1795.77
150	5.300	-7.837	10.058	1.567	3.208	0.629	1723.61
151	5.400	-7.075	9.089	1.490	3.049	0.615	1668.90
152	5.500	-6.426	8.346	1.433	2.912	0.602	1623.42
153	5.600	-5.865	7.785	1.393	2.794	0.588	1585.91
154	5.700	-5.360	7.346	1.366	2.688	0.574	1553.11
155	5.800	-4.943	7.013	1.349	2.600	0.561	1528.73
156	5.900	-4.611	6.776	1.339	2.531	0.549	1513.36

157	6.000	-4.261	6.551	1.333	2.457	0.536	1494.40
158	-----						
159	47	0.315	4	(mx, y, iy)			
160	1.500	11.585	0.000	3.404	0.000	0.298	0.00
161	1.600	11.945	0.000	3.456	0.000	0.304	0.00
162	1.700	12.312	0.000	3.509	0.000	0.310	0.00
163	1.800	12.901	0.058	3.592	0.008	0.319	1.46
164	1.864	13.423	0.1	3.664	0.014		
165	1.900	13.309	0.812	3.650	0.111	0.325	21.43
166	2.000	13.597	1.070	3.690	0.145	0.330	29.38
167	2.100	14.036	1.250	3.750	0.167	0.336	35.47
168	2.200	14.516	1.543	3.815	0.202	0.343	45.08
169	2.300	14.937	1.755	3.872	0.227	0.349	52.83
170	2.400	15.495	2.038	3.945	0.258	0.356	62.83
171	2.500	16.167	2.460	4.032	0.305	0.365	77.30
172	2.600	16.963	3.037	4.135	0.367	0.367	96.76
173	2.700	17.928	3.794	4.258	0.446	0.388	121.93
174	2.800	19.089	4.900	4.404	0.556	0.403	157.89
175	2.900	20.478	6.614	4.582	0.722	0.421	212.14
176	3.000	21.832	9.680	4.781	1.012	0.445	307.84
177	3.100	20.854	15.031	4.825	1.558	0.469	489.44
178	3.200	16.329	16.746	4.456	1.879	0.465	609.42
179	3.300	13.867	17.334	4.246	2.041	0.464	682.67
180	3.400	10.827	16.737	3.922	2.134	0.455	735.39
181	3.500	9.653	15.298	3.724	2.054	0.439	728.58
182	3.600	9.242	14.445	3.633	1.988	0.428	725.50
183	3.700	9.094	13.968	3.589	1.946	0.422	729.80
184	3.800	9.095	13.734	3.575	1.921	0.419	739.75
185	3.900	9.212	13.739	3.588	1.914	0.419	756.76
186	4.000	9.427	13.973	3.625	1.927	0.422	781.41
187	4.100	9.723	14.492	3.686	1.966	0.429	816.92
188	4.200	10.065	15.387	3.772	2.040	0.440	868.37
189	4.300	10.362	16.868	3.883	2.172	0.456	946.63
190	4.400	10.266	19.139	3.999	2.393	0.479	1067.23
191	4.500	9.029	22.204	4.062	2.733	0.509	1246.64
192	4.600	5.766	25.299	3.982	3.177	0.544	1481.12
193	4.700	0.383	26.540	3.669	3.617	0.579	1722.91
194	4.800	-4.850	24.805	3.196	3.881	0.609	1888.25
195	4.900	-8.451	21.238	2.684	3.957	0.633	1965.08
196	5.000	-9.954	16.908	2.198	3.845	0.648	1948.84
197	5.100	-9.460	13.534	1.878	3.604	0.647	1862.86
198	5.200	-8.520	11.454	1.696	3.376	0.637	1779.44
199	5.300	-7.656	10.078	1.581	3.187	0.624	1712.04
200	5.400	-6.940	9.074	1.497	3.030	0.612	1658.54
201	5.500	-6.308	8.313	1.437	2.893	0.598	1613.01
202	5.600	-5.765	7.734	1.393	2.776	0.585	1575.68
203	5.700	-5.255	7.296	1.367	2.669	0.570	1541.99
204	5.800	-4.814	6.967	1.352	2.577	0.556	1514.99
205	5.900	-4.471	6.698	1.338	2.502	0.544	1496.52
206	6.000	-4.156	6.583	1.347	2.443	0.531	1486.00
207	-----						
208	46	0.419	5	(mx, y, iy)			
209	1.500	11.160	0.000	3.341	0.000	0.291	0.00

210	1.600	11.412	0.000	3.378	0.000	0.295	0.00
211	1.700	11.709	0.000	3.422	0.000	0.300	0.00
212	1.800	12.106	0.000	3.479	0.000	0.306	0.00
213	1.900	12.669	0.018	3.559	0.003	0.315	0.49
214	2.000	13.423	0.431	3.664	0.059	0.326	11.91
215	2.100	13.578	0.735	3.686	0.100	0.329	21.21
216	2.200	14.022	1.003	3.747	0.134	0.335	29.86
217	2.300	14.562	1.357	3.820	0.178	0.343	41.40
218	2.400	15.015	1.700	3.881	0.219	0.350	53.29
219	2.500	15.582	2.120	3.957	0.268	0.353	67.88
220	2.600	16.279	2.581	4.047	0.319	0.367	84.03
221	2.700	17.103	3.202	4.154	0.385	0.378	105.49
222	2.800	18.100	4.037	4.280	0.472	0.391	133.82
223	2.900	19.273	5.279	4.430	0.596	0.406	175.12
224	3.000	20.591	7.236	4.605	0.786	0.425	238.89
225	3.100	21.579	10.694	4.778	1.119	0.448	351.61
226	3.200	19.457	15.439	4.706	1.640	0.466	532.03
227	3.300	15.873	16.459	4.401	1.870	0.461	625.45
228	3.400	13.237	17.043	4.172	2.042	0.460	703.85
229	3.500	10.814	16.101	3.887	2.071	0.448	734.87
230	3.600	9.940	14.982	3.736	2.005	0.435	731.61
231	3.700	9.622	14.365	3.668	1.958	0.427	734.32
232	3.800	9.516	14.059	3.640	1.931	0.424	743.92
233	3.900	9.549	14.005	3.640	1.924	0.423	760.47
234	4.000	9.696	14.201	3.667	1.936	0.425	785.08
235	4.100	9.942	14.663	3.719	1.971	0.431	819.31
236	4.200	10.229	15.482	3.794	2.040	0.441	868.66
237	4.300	10.519	16.846	3.897	2.161	0.456	941.92
238	4.400	10.530	18.973	4.014	2.363	0.477	1053.94
239	4.500	9.587	22.083	4.103	2.691	0.507	1227.63
240	4.600	6.468	25.594	4.054	3.157	0.543	1471.88
241	4.700	0.644	27.217	3.733	3.646	0.582	1736.73
242	4.800	-5.043	25.014	3.200	3.909	0.611	1901.83
243	4.900	-8.234	21.217	2.695	3.937	0.630	1955.15
244	5.000	-9.614	17.074	2.234	3.822	0.643	1936.79
245	5.100	-9.238	13.861	1.926	3.598	0.642	1860.13
246	5.200	-8.428	11.775	1.740	3.384	0.633	1783.80
247	5.300	-7.643	10.329	1.613	3.201	0.622	1719.58
248	5.400	-6.964	9.277	1.523	3.047	0.611	1667.58
249	5.500	-6.334	8.469	1.456	2.908	0.598	1621.01
250	5.600	-5.765	7.828	1.406	2.783	0.584	1579.54
251	5.700	-5.259	7.365	1.377	2.675	0.570	1545.40
252	5.800	-4.787	6.985	1.357	2.574	0.555	1513.42
253	5.900	-4.465	6.767	1.350	2.507	0.543	1499.39
254	6.000	-4.124	6.602	1.353	2.440	0.529	1483.96
255	-----						
256	46	0.491	6	(mx, y, iy)			
257	1.500	10.780	0.000	3.283	0.000	0.284	0.00
258	1.600	11.080	0.000	3.329	0.000	0.289	0.00
259	1.700	11.344	0.000	3.368	0.000	0.294	0.00
260	1.800	11.676	0.000	3.417	0.000	0.299	0.01
261	1.900	12.089	0.000	3.477	0.000	0.306	0.02
262	2.000	12.659	0.016	3.558	0.002	0.315	0.46

263	2.100	13.423	0.647	3.665	0.088	0.327	18.80
264	2.200	13.639	0.985	3.696	0.133	0.330	29.72
265	2.300	14.115	1.234	3.761	0.164	0.337	38.25
266	2.400	14.685	1.571	3.838	0.205	0.345	49.79
267	2.500	15.176	1.914	3.903	0.245	0.352	62.12
268	2.600	15.797	2.331	3.985	0.292	0.361	77.07
269	2.700	16.525	2.900	4.081	0.355	0.371	97.24
270	2.800	17.411	3.596	4.195	0.429	0.382	121.66
271	2.900	18.445	4.623	4.328	0.534	0.396	156.98
272	3.000	19.629	6.132	4.483	0.684	0.413	207.96
273	3.100	20.801	8.624	4.654	0.926	0.433	291.11
274	3.200	20.801	12.735	4.753	1.340	0.455	434.48
275	3.300	17.419	15.823	4.525	1.748	0.461	584.80
276	3.400	14.746	16.502	4.294	1.922	0.458	662.21
277	3.500	12.074	16.529	4.034	2.049	0.454	726.82
278	3.600	10.534	15.419	3.822	2.017	0.440	736.17
279	3.700	9.992	14.670	3.724	1.969	0.431	738.60
280	3.800	9.771	14.294	3.680	1.942	0.427	748.01
281	3.900	9.737	14.190	3.671	1.933	0.425	764.12
282	4.000	9.821	14.346	3.688	1.945	0.427	788.49
283	4.100	9.995	14.768	3.730	1.980	0.433	822.67
284	4.200	10.237	15.540	3.798	2.046	0.442	871.00
285	4.300	10.502	16.815	3.894	2.159	0.456	941.02
286	4.400	10.547	18.847	4.009	2.351	0.476	1048.33
287	4.500	9.752	21.915	4.107	2.668	0.505	1216.88
288	4.600	6.678	25.524	4.072	3.147	0.543	1467.13
289	4.700	0.636	27.202	3.731	3.645	0.582	1736.48
290	4.800	-5.044	24.850	3.187	3.899	0.611	1896.85
291	4.900	-8.024	20.971	2.686	3.904	0.627	1938.84
292	5.000	-9.278	17.038	2.250	3.787	0.639	1919.09
293	5.100	-9.003	13.967	1.951	3.579	0.637	1850.21
294	5.200	-8.301	11.910	1.763	3.378	0.630	1780.31
295	5.300	-7.573	10.444	1.632	3.199	0.620	1718.78
296	5.400	-6.923	9.330	1.532	3.045	0.609	1666.52
297	5.500	-6.293	8.487	1.462	2.903	0.596	1618.56
298	5.600	-5.733	7.849	1.412	2.780	0.583	1577.75
299	5.700	-5.205	7.351	1.379	2.666	0.568	1540.12
300	5.800	-4.755	7.018	1.364	2.572	0.553	1512.15
301	5.900	-4.344	6.790	1.363	2.490	0.537	1489.38
302	6.000	-3.983	6.608	1.366	2.418	0.523	1470.81
303	-----						
304	46	0.590	7	(mx, y, iy)			
305	1.500	10.480	0.000	3.237	0.000	0.279	0.00
306	1.600	10.721	0.000	3.274	0.000	0.283	0.00
307	1.700	10.973	0.000	3.313	0.000	0.288	0.00
308	1.800	11.247	0.000	3.354	0.000	0.292	0.00
309	1.900	11.591	0.000	3.405	0.000	0.298	0.00
310	2.000	12.017	0.000	3.467	0.000	0.305	0.01
311	2.100	12.575	0.034	3.546	0.005	0.314	1.03
312	2.200	13.380	0.458	3.658	0.063	0.326	13.95
313	2.300	13.599	0.931	3.690	0.126	0.329	29.43
314	2.400	14.097	1.181	3.758	0.157	0.337	38.23
315	2.500	14.682	1.574	3.837	0.205	0.345	51.97

316	2.600	15.208	2.047	3.909	0.262	0.353	69.00
317	2.700	15.837	2.532	3.992	0.317	0.362	86.80
318	2.800	16.600	3.140	4.092	0.384	0.372	108.87
319	2.900	17.493	3.936	4.208	0.468	0.384	137.44
320	3.000	18.517	5.070	4.343	0.584	0.399	177.51
321	3.100	19.653	6.784	4.497	0.754	0.416	237.00
322	3.200	20.560	9.557	4.649	1.028	0.436	333.35
323	3.300	19.663	13.530	4.665	1.450	0.454	485.03
324	3.400	16.542	15.536	4.429	1.754	0.456	604.41
325	3.500	14.137	16.255	4.224	1.924	0.455	682.65
326	3.600	11.804	15.923	3.977	2.002	0.447	730.58
327	3.700	10.713	15.077	3.822	1.973	0.437	739.80
328	3.800	10.287	14.581	3.750	1.944	0.431	748.73
329	3.900	10.131	14.417	3.725	1.935	0.428	765.00
330	4.000	10.113	14.518	3.729	1.947	0.430	789.30
331	4.100	10.210	14.870	3.758	1.978	0.434	822.15
332	4.200	10.403	15.554	3.815	2.038	0.442	867.72
333	4.300	10.647	16.723	3.903	2.142	0.455	933.67
334	4.400	10.746	18.612	4.015	2.318	0.474	1033.77
335	4.500	10.194	21.592	4.127	2.616	0.502	1193.05
336	4.600	7.325	25.601	4.120	3.107	0.541	1448.53
337	4.700	1.071	27.219	3.762	3.617	0.579	1723.21
338	4.800	-4.574	24.901	3.221	3.866	0.607	1880.90
339	4.900	-7.553	21.268	2.740	3.881	0.623	1927.50
340	5.000	-8.921	17.385	2.304	3.772	0.634	1911.84
341	5.100	-8.797	14.375	2.007	3.581	0.633	1851.25
342	5.200	-8.246	12.245	1.805	3.392	0.627	1787.75
343	5.300	-7.589	10.682	1.661	3.217	0.619	1727.95
344	5.400	-6.945	9.504	1.553	3.059	0.609	1674.41
345	5.500	-6.321	8.600	1.475	2.915	0.596	1625.05
346	5.600	-5.732	7.920	1.422	2.785	0.582	1580.61
347	5.700	-5.195	7.413	1.389	2.669	0.567	1542.06
348	5.800	-4.701	7.030	1.370	2.565	0.551	1507.87
349	5.900	-4.301	6.810	1.370	2.485	0.535	1486.39
350	6.000	-3.936	6.704	1.385	2.420	0.520	1471.56
351	-----						
352	46	0.700	8	(mx, y, iy)			
353	1.500	9.940	0.000	3.153	0.000	0.269	0.00
354	1.600	10.161	0.000	3.188	0.000	0.273	0.00
355	1.700	10.398	0.000	3.225	0.000	0.277	0.00
356	1.800	10.636	0.000	3.261	0.000	0.282	0.00
357	1.900	10.928	0.000	3.306	0.000	0.287	0.00
358	2.000	11.294	0.000	3.361	0.000	0.293	0.00
359	2.100	11.728	0.001	3.425	0.000	0.300	0.03
360	2.200	12.252	0.003	3.500	0.000	0.309	0.09
361	2.300	12.924	0.016	3.595	0.002	0.319	0.51
362	2.400	13.653	0.513	3.696	0.069	0.330	16.89
363	2.500	14.012	0.969	3.746	0.129	0.335	32.78
364	2.600	14.582	1.408	3.823	0.184	0.344	48.54
365	2.700	15.200	1.918	3.906	0.245	0.353	67.19
366	2.800	15.806	2.446	3.987	0.307	0.361	87.05
367	2.900	16.538	3.058	4.084	0.374	0.371	110.04
368	3.000	17.393	3.857	4.196	0.460	0.383	139.75

369	3.100	18.378	4.965	4.325	0.574	0.397	180.35
370	3.200	19.450	6.576	4.471	0.735	0.413	238.51
371	3.300	20.334	9.049	4.615	0.980	0.432	327.96
372	3.400	19.925	12.658	4.665	1.357	0.450	467.51
373	3.500	17.454	15.104	4.502	1.678	0.456	595.12
374	3.600	15.128	16.217	4.319	1.877	0.457	685.06
375	3.700	12.864	16.355	4.103	1.993	0.453	747.43
376	3.800	11.550	15.837	3.947	2.006	0.446	772.81
377	3.900	10.928	15.538	3.868	2.009	0.442	793.97
378	4.000	10.620	15.516	3.836	2.023	0.442	820.09
379	4.100	10.487	15.765	3.835	2.055	0.444	854.10
380	4.200	10.502	16.330	3.868	2.111	0.450	898.74
381	4.300	10.595	17.349	3.932	2.206	0.461	961.51
382	4.400	10.632	19.053	4.028	2.365	0.478	1054.80
383	4.500	10.160	21.908	4.142	2.645	0.504	1206.30
384	4.600	7.253	26.106	4.144	3.150	0.544	1468.60
385	4.700	0.897	27.338	3.758	3.637	0.581	1732.65
386	4.800	-4.518	24.762	3.214	3.853	0.606	1874.51
387	4.900	-7.292	21.512	2.777	3.873	0.620	1923.76
388	5.000	-8.809	17.839	2.354	3.788	0.632	1919.97
389	5.100	-8.906	14.834	2.049	3.620	0.634	1871.32
390	5.200	-8.526	12.599	1.829	3.445	0.632	1815.84
391	5.300	-7.924	10.863	1.662	3.269	0.626	1756.01
392	5.400	-7.215	9.572	1.545	3.098	0.616	1695.93
393	5.500	-6.541	8.613	1.462	2.946	0.603	1642.26
394	5.600	-5.908	7.903	1.407	2.809	0.589	1594.16
395	5.700	-5.337	7.391	1.375	2.688	0.573	1553.18
396	5.800	-4.796	7.046	1.365	2.581	0.554	1517.15
397	5.900	-4.348	6.811	1.366	2.493	0.537	1490.74
398	6.000	-3.991	6.683	1.377	2.426	0.523	1475.64
399	-----						
400	46	0.804	9	(mx, y, iy)			
401	1.500	9.761	0.000	3.124	0.000	0.265	0.00
402	1.600	9.902	0.000	3.147	0.000	0.268	0.00
403	1.700	10.068	0.000	3.173	0.000	0.271	0.00
404	1.800	10.251	0.000	3.202	0.000	0.275	0.00
405	1.900	10.472	0.000	3.236	0.000	0.279	0.00
406	2.000	10.739	0.000	3.277	0.000	0.283	0.00
407	2.100	11.038	0.000	3.322	0.000	0.289	0.00
408	2.200	11.408	0.000	3.378	0.000	0.295	0.00
409	2.300	11.834	0.019	3.440	0.003	0.302	0.64
410	2.400	12.382	0.025	3.519	0.004	0.311	0.87
411	2.500	13.217	0.095	3.635	0.013	0.323	3.30
412	2.600	13.964	0.778	3.738	0.104	0.334	27.42
413	2.700	14.315	1.217	3.787	0.161	0.340	43.96
414	2.800	14.948	1.586	3.872	0.205	0.349	58.12
415	2.900	15.613	2.190	3.961	0.276	0.358	81.26
416	3.000	16.281	2.859	4.050	0.353	0.368	107.31
417	3.100	17.072	3.632	4.155	0.437	0.379	137.32
418	3.200	18.001	4.625	4.277	0.541	0.392	175.38
419	3.300	19.007	6.042	4.413	0.685	0.407	228.97
420	3.400	20.017	8.123	4.562	0.890	0.425	306.82
421	3.500	20.339	11.193	4.667	1.199	0.444	425.45

422	3.600	18.845	14.405	4.613	1.561	0.456	569.68
423	3.700	16.603	16.240	4.462	1.820	0.462	682.44
424	3.800	14.152	17.181	4.267	2.013	0.463	775.50
425	3.900	12.255	17.059	4.078	2.092	0.459	826.82
426	4.000	11.207	16.793	3.962	2.119	0.456	859.20
427	4.100	10.643	16.737	3.904	2.144	0.455	890.89
428	4.200	10.392	17.002	3.893	2.183	0.458	929.51
429	4.300	10.334	17.723	3.928	2.256	0.465	983.42
430	4.400	10.323	19.127	4.004	2.389	0.479	1065.33
431	4.500	9.941	21.704	4.112	2.639	0.503	1203.83
432	4.600	7.082	25.692	4.107	3.128	0.542	1458.44
433	4.700	1.235	26.869	3.751	3.582	0.576	1706.48
434	4.800	-3.720	24.345	3.233	3.765	0.597	1831.69
435	4.900	-6.524	21.615	2.833	3.815	0.612	1894.58
436	5.000	-8.274	18.256	2.426	3.763	0.625	1907.01
437	5.100	-8.758	15.338	2.110	3.635	0.631	1878.88
438	5.200	-8.628	12.909	1.857	3.475	0.633	1831.74
439	5.300	-8.089	10.939	1.661	3.293	0.629	1769.26
440	5.400	-7.300	9.489	1.528	3.104	0.619	1699.08
441	5.500	-6.517	8.495	1.447	2.935	0.604	1636.04
442	5.600	-5.837	7.808	1.399	2.792	0.587	1584.53
443	5.700	-5.237	7.307	1.370	2.667	0.570	1540.88
444	5.800	-4.722	6.931	1.354	2.560	0.552	1505.06
445	5.900	-4.267	6.729	1.360	2.473	0.534	1479.16
446	6.000	-3.931	6.589	1.368	2.409	0.520	1464.84

447 -----

448 =h==

6.6.8 W.GA_P

```

1 -----
2 Optical Properties of:   Gallium Phosphide (GaP)
3
4 1)   Handbook of Optical Constants,
5       edited by Edward D. Palik,
6       (Academic Press, Inc., Orlando, 1985)
7
8 2)   D.E. Aspnes & A.A. Studna,
9       Physical Review B, Volume 27, Number 2, 1983 January 15.
10      Pages: 985-1009.
11
12 -----
13 E(eV),      n,      k,      R,      alpha*1.0E3 (cm**-1)
14 -----
15 =h==          " indicate end of header information
16 156           " quantity of lines of data
17 1.500      3.178      0.0      0.272      0.0
18 1.54       3.191      0.0
19 1.600      3.209      0.0      0.275      0.0
20 1.64       3.219      0.0
21 1.700      3.234      0.0      0.278      0.0
22 1.74       3.245      0.0
23 1.800      3.262      0.0      0.282      0.0
24 1.84       3.275      0.0
25 1.900      3.295      0.0      0.286      0.0
26 1.94       3.311      0.0
27 2.000      3.334      0.0      0.290      0.0
28 2.04       3.350      0.0
29 2.100      3.375      0.0      0.295      0.01
30 2.14       3.393      0.0
31 2.18       3.411      2.8E-7
32 2.200      3.421      1.4E-6      0.3      0.04
33 2.22       3.430      3.1E-6
34 2.24       3.441      2.7E-6
35 2.26       3.452      6.2E-6
36 2.28       3.463      1.3E-4
37 2.300      3.474      2.5E-4      0.306      0.36
38 2.34       3.497      5.5E-4
39 2.400      3.535      1.1E-3      0.312      0.86
40 2.44       3.561      1.6E-3
41 2.48       3.590      2.47E-3
42 2.500      3.605      2.54E-3      0.320      1.63
43 2.54       3.638      3.1E-3
44 2.600      3.691      5.5E-3      0.329      2.94
45 2.64       3.730      1.5E-2
46 2.700      3.805      2.7E-2      0.341      7.52
47 2.72       3.835      3.5E-2
48 2.74       3.869      5.7E-2
49 2.76       3.896      8.5E-2
50 2.78       3.904      0.103

```


51	2.800	3.919	0.118	0.352	33.42
52	2.82	3.936	0.135		
53	2.84	3.952	0.152		
54	2.86	3.964	0.165		
55	2.88	3.976	0.176		
56	2.900	3.990	0.183	0.360	53.90
57	2.92	4.006	0.194		
58	2.94	4.023	0.202		
59	2.96	4.041	0.208		
60	2.98	4.060	0.218		
61	3.000	4.081	0.224	0.369	68.26
62	3.02	4.102	0.233		
63	3.04	4.124	0.244		
64	3.06	4.147	0.253		
65	3.08	4.171	0.264		
66	3.100	4.196	0.275	0.380	86.28
67	3.12	4.222	0.285		
68	3.14	4.249	0.298		
69	3.16	4.278	0.310		
70	3.18	4.308	0.323		
71	3.200	4.339	0.337	0.394	109.25
72	3.22	4.372	0.353		
73	3.24	4.406	0.369		
74	3.26	4.442	0.388		
75	3.28	4.479	0.407		
76	3.300	4.518	0.426	0.410	142.64
77	3.32	4.560	0.449		
78	3.34	4.604	0.475		
79	3.36	4.651	0.503		
80	3.38	4.700	0.534		
81	3.400	4.751	0.568	0.431	195.80
82	3.42	4.805	0.605		
83	3.44	4.861	0.649		
84	3.46	4.920	0.697		
85	3.48	4.983	0.752		
86	3.500	5.050	0.819	0.458	290.40
87	3.52	5.121	0.893		
88	3.54	5.194	0.982		
89	3.56	5.268	1.089		
90	3.58	5.339	1.217		
91	3.600	5.406	1.368	0.496	499.04
92	3.62	5.454	1.550		
93	3.64	5.472	1.766		
94	3.66	5.437	2.010		
95	3.68	5.328	2.250		
96	3.700	5.149	2.451	0.530	919.21
97	3.72	4.927	2.585		
98	3.74	4.700	2.646		
99	3.76	4.497	2.649		
100	3.78	4.328	2.615		
101	3.800	4.196	2.562	0.500	986.69
102	3.82	4.095	2.502		
103	3.84	4.021	2.443		

104	3.86	3.966	2.389		
105	3.88	3.923	2.343		
106	3.900	3.890	2.303	0.467	910.55
107	3.94	3.840	2.240		
108	4.000	3.790	2.171	0.452	880.10
109	4.04	3.769	2.137		
110	4.100	3.752	2.100	0.444	872.59
111	4.14	3.748	2.082		
112	4.200	3.754	2.063	0.441	878.38
113	4.24	3.765	2.057		
114	4.300	3.792	2.058	0.442	896.99
115	4.34	3.817	2.066		
116	4.400	3.867	2.090	0.449	932.14
117	4.44	3.907	2.117		
118	4.500	3.978	2.180	0.461	994.27
119	4.54	4.031	2.241		
120	4.600	4.113	2.371	0.482	1105.61
121	4.62	4.137	2.427		
122	4.64	4.158	2.491		
123	4.66	4.173	2.560		
124	4.68	4.181	2.634		
125	4.700	4.181	2.712	0.511	1291.94
126	4.72	4.173	2.791		
127	4.74	4.157	2.871		
128	4.76	4.132	2.949		
129	4.78	4.100	3.024		
130	4.800	4.062	3.096	0.539	1506.17
131	4.82	4.018	3.162		
132	4.84	3.970	3.218		
133	4.86	3.923	3.269		
134	4.88	3.880	3.316		
135	4.900	3.844	3.358	0.557	1667.57
136	4.92	3.806	3.404		
137	4.94	3.774	3.454		
138	4.96	3.739	3.509		
139	4.98	3.701	3.567		
140	5.000	3.661	3.631	0.580	1839.99
141	5.02	3.615	3.698		
142	5.04	3.561	3.768		
143	5.06	3.498	3.839		
144	5.08	3.424	3.909		
145	5.100	3.342	3.975	0.614	2054.74
146	5.12	3.248	4.036		
147	5.14	3.144	4.086		
148	5.16	3.036	4.123		
149	5.18	2.930	4.150		
150	5.200	2.825	4.170	0.647	2197.82
151	5.22	2.718	4.185		
152	5.24	2.607	4.197		
153	5.26	2.490	4.201		
154	5.28	2.368	4.192		
155	5.300	2.248	4.168	0.678	2239.10
156	5.32	2.134	4.128		

157	5.34	2.028	4.077		
158	5.36	1.936	4.019		
159	5.38	1.851	3.955		
160	5.400	1.778	3.889	0.689	2128.87
161	5.44	1.660	3.752		
162	5.500	1.543	3.556	0.677	1982.53
163	5.54	1.494	3.441		
164	5.600	1.444	3.297	0.657	1871.33
165	5.64	1.418	3.211		
166	5.700	1.385	3.096	0.637	1768.84
167	5.74	1.368	3.028		
168	5.800	1.348	2.934	0.618	1724.82
169	5.84	1.342	2.882		
170	5.900	1.327	2.803	0.600	1676.14
171	5.94	1.327	2.766		
172	6.000	1.309	2.690	0.583	1635.71
173	=h==				

· indicate end of information

6.6.9 W.GA_SB

1	-----						
2	Optical Properties of: Gallium Antimonide (GaSb)						
3							
4	D.E. Aspnes & A.A. Studna,						
5	Physical Review B, Volume 27, Number 2, 1983, January, 15.						
6	Pages: 985-1009.						
7							
8	-----						
9	E(eV),	<e1>,	<e2>,	n,	k,	R,	alpha*1.0E3 (cm**-1)
10	-----						
11	=h==	" indicate end of header information					
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13	1.500	19.135	3.023	4.388	0.344	0.398	52.37
14	1.600	20.137	3.752	4.507	0.416	0.409	67.51
15	1.700	21.322	4.503	4.643	0.485	0.421	83.56
16	1.800	22.826	5.889	4.817	0.611	0.437	111.53
17	1.900	24.836	8.373	5.052	0.829	0.458	159.59
18	2.000	25.545	14.442	5.239	1.378	0.487	279.43
19	2.100	18.883	16.963	4.705	1.803	0.474	383.74
20	2.200	17.386	15.794	4.521	1.747	0.461	389.54
21	2.300	16.980	16.069	4.492	1.789	0.461	416.97
22	2.400	16.521	17.708	4.513	1.962	0.473	477.22
23	2.500	13.367	19.705	4.312	2.285	0.484	579.07
24	2.600	10.676	18.172	3.984	2.280	0.470	600.94
25	2.700	9.828	16.966	3.836	2.211	0.457	605.14
26	2.800	9.484	16.216	3.760	2.157	0.449	612.05
27	2.900	9.399	15.810	3.728	2.121	0.445	623.34
28	3.000	9.479	15.738	3.732	2.109	0.444	641.20
29	3.100	9.628	16.070	3.766	2.134	0.448	670.45
30	3.200	9.558	16.797	3.800	2.210	0.456	716.82
31	3.300	9.121	17.656	3.808	2.319	0.465	775.62
32	3.400	8.490	18.440	3.794	2.430	0.475	837.48
33	3.500	7.852	19.267	3.785	2.545	0.485	902.86
34	3.600	7.011	20.306	3.774	2.690	0.497	981.54
35	3.700	5.853	21.453	3.748	2.862	0.512	1073.44
36	3.800	4.281	22.719	3.701	3.069	0.530	1182.10
37	3.900	2.058	24.057	3.620	3.323	0.553	1313.68
38	4.000	-1.374	25.138	3.450	3.643	0.583	1477.21
39	4.100	-6.203	24.648	3.100	3.976	0.620	1652.40
40	4.200	-10.699	20.831	2.522	4.130	0.658	1758.30
41	4.300	-11.435	15.607	1.989	3.923	0.673	1709.93
42	4.400	-10.196	12.500	1.723	3.628	0.665	1618.09
43	4.500	-8.989	10.763	1.586	3.392	0.651	1547.17
44	4.600	-8.031	9.642	1.503	3.208	0.637	1495.68
45	4.700	-7.249	8.823	1.444	3.055	0.623	1455.44
46	4.800	-6.594	8.244	1.408	2.928	0.608	1424.76
47	4.900	-6.079	7.846	1.387	2.829	0.595	1405.00
48	5.000	-5.693	7.529	1.369	2.751	0.585	1394.02
49	5.100	-5.365	7.290	1.358	2.685	0.575	1387.91
50	5.200	-5.156	7.173	1.356	2.645	0.568	1394.03

51	5.300	-5.151	7.099	1.345	2.638	0.568	1417.39
52	5.400	-5.353	6.890	1.299	2.653	0.578	1452.17
53	5.500	-5.527	6.410	1.212	2.645	0.592	1474.51
54	5.600	-5.497	5.866	1.127	2.602	0.601	1476.67
55	5.700	-5.297	5.385	1.062	2.535	0.602	1464.56
56	5.800	-5.102	5.070	1.022	2.479	0.601	1457.65
57	5.900	-5.002	4.814	0.985	2.444	0.603	1461.49
58	6.000	-4.962	4.520	0.935	2.416	0.610	1469.28
59	=h==	* indicate end of information					

6.6.10 W.IN_AS

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1 -----
2 Optical Properties of:   Indium Arsenide (InAs)
3
4 D.E. Aspnes & A.A. Studna,
5 Physical Review B, Volume 27, Number 2, 1983, January, 15.
6 Pages: 985-1009.
7
8 -----
9 E(eV),      <e1>,      <e2>,      n,      k,      R,      alpha*1.0E3 (cm**-1)
10 -----
11 =h==          " indicate end of header information
12 46            " quantity of lines of data
13 1.500        13.605      3.209      3.714      0.432      0.337      65.69
14 1.600        13.884      3.478      3.755      0.463      0.342      75.11
15 1.700        14.181      3.744      3.798      0.493      0.347      84.94
16 1.800        14.545      4.083      3.851      0.530      0.353      96.72
17 1.900        15.015      4.481      3.917      0.572      0.361     110.16
18 2.000        15.558      5.062      3.995      0.634      0.370     128.43
19 2.100        16.205      5.820      4.088      0.712      0.380     151.51
20 2.200        16.957      6.905      4.199      0.822      0.394     183.33
21 2.300        17.776      8.582      4.331      0.991      0.411     230.98
22 2.400        18.298     11.458      4.466      1.283      0.433     312.08
23 2.500        15.856     15.592      4.364      1.786      0.454     452.64
24 2.600        12.611     15.160      4.021      1.885      0.441     496.84
25 2.700        11.229     15.766      3.911      2.016      0.445     551.66
26 2.800         8.276     16.010      3.626      2.208      0.448     626.53
27 2.900         6.603     14.211      3.337      2.129      0.428     625.87
28 3.000         6.083     13.003      3.197      2.034      0.412     618.46
29 3.100         5.831     12.162      3.108      1.957      0.400     614.80
30 3.200         5.736     11.540      3.051      1.891      0.389     613.30
31 3.300         5.735     11.082      3.018      1.836      0.381     614.18
32 3.400         5.820     10.753      3.004      1.790      0.375     616.84
33 3.500         5.973     10.550      3.008      1.754      0.371     622.13
34 3.600         6.197     10.471      3.030      1.728      0.370     630.47
35 3.700         6.478     10.529      3.069      1.715      0.370     643.29
36 3.800         6.835     10.754      3.129      1.719      0.374     661.95
37 3.900         7.254     11.187      3.208      1.743      0.382     689.18
38 4.000         7.744     11.919      3.313      1.799      0.393     729.23
39 4.100         8.273     13.130      3.449      1.903      0.411     791.03
40 4.200         8.663     15.173      3.615      2.099      0.437     893.42
41 4.300         8.000     18.639      3.761      2.478      0.478    1080.14
42 4.400         4.024     22.171      3.644      3.042      0.527    1356.76
43 4.500        -1.663     22.006      3.194      3.445      0.566    1571.19
44 4.600        -5.509     19.372      2.705      3.581      0.593    1669.74
45 4.700        -7.921     15.762      2.205      3.575      0.617    1703.11
46 4.800        -7.961     12.077      1.803      3.349      0.622    1629.16
47 4.900        -6.905      9.909      1.608      3.081      0.605    1530.10
48 5.000        -5.923      8.752      1.524      2.871      0.583    1455.26
49 5.100        -5.264      8.107      1.484      2.732      0.565    1412.38
50 5.200        -4.942      7.600      1.436      2.646      0.556    1394.86

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51	5.300	-4.665	6.980	1.366	2.555	0.550	1372.78
52	5.400	-4.278	6.425	1.312	2.449	0.537	1340.56
53	5.500	-3.851	6.008	1.282	2.344	0.521	1306.62
54	5.600	-3.424	5.738	1.276	2.248	0.501	1275.94
55	5.700	-3.006	5.595	1.293	2.163	0.479	1249.73
56	5.800	-2.642	5.602	1.333	2.102	0.459	1235.70
57	5.900	-2.430	5.764	1.383	2.084	0.448	1246.25
58	6.000	-2.403	6.055	1.434	2.112	0.448	1284.15
59	=h==	" indicate end of information					

6.6.11 W.IN_P

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1 -----
2 Optical Properties of: Indium Phosphide (InP)
3
4 D.E. Aspnes & A.A. Studna,
5 Physical Review B, Volume 27, Number 2, 1983, January, 15.
6 Pages: 985-1009.
7
8 -----
9 E(eV),      <e1>,      <e2>,      n,      k,      R,      alpha*1.0E3 (cm**-1)
10 -----
11 =h==          " indicate end of header information
12 46            " quantity of lines of data
13 1.500      11.904      1.400      3.456      0.203      0.305      30.79
14 1.600      11.972      1.509      3.467      0.218      0.307      35.30
15 1.700      12.022      1.680      3.476      0.242      0.308      41.64
16 1.800      12.120      1.889      3.492      0.270      0.310      49.34
17 1.900      12.284      2.062      3.517      0.293      0.313      56.44
18 2.000      12.493      2.252      3.549      0.317      0.317      64.32
19 2.100      12.734      2.488      3.585      0.347      0.322      73.87
20 2.200      13.026      2.755      3.629      0.380      0.327      84.65
21 2.300      13.382      3.060      3.682      0.416      0.333      96.89
22 2.400      13.812      3.425      3.745      0.457      0.341      111.25
23 2.500      14.313      3.904      3.818      0.511      0.349      129.56
24 2.600      14.899      4.524      3.903      0.579      0.360      152.71
25 2.700      15.585      5.337      4.004      0.667      0.372      182.41
26 2.800      16.365      6.482      4.121      0.786      0.386      223.21
27 2.900      17.188      8.205      4.256      0.964      0.404      283.32
28 3.000      17.759      10.962      4.395      1.247      0.427      379.23
29 3.100      18.483      15.325      4.415      1.735      0.454      545.30
30 3.200      11.211      17.043      3.976      2.143      0.458      695.23
31 3.300      7.911      15.797      3.576      2.209      0.446      738.76
32 3.400      6.639      13.592      3.299      2.060      0.419      709.95
33 3.500      6.400      12.443      3.193      1.948      0.403      691.21
34 3.600      6.312      11.731      3.133      1.872      0.391      683.12
35 3.700      6.330      11.266      3.103      1.816      0.383      680.92
36 3.800      6.432      10.974      3.095      1.773      0.378      682.96
37 3.900      6.616      10.841      3.108      1.744      0.376      689.47
38 4.000      6.874      10.871      3.141      1.730      0.376      701.54
39 4.100      7.205      11.088      3.196      1.735      0.380      720.91
40 4.200      7.620      11.539      3.275      1.762      0.387      750.02
41 4.300      8.119      12.358      3.384      1.826      0.400      795.80
42 4.400      8.644      13.739      3.527      1.948      0.419      868.69
43 4.500      8.891      16.161      3.697      2.186      0.449      996.95
44 4.600      7.484      20.039      3.800      2.637      0.493      1229.49
45 4.700      2.292      22.948      3.560      3.223      0.543      1535.24
46 4.800      -3.469      20.989      2.984      3.517      0.577      1711.26
47 4.900      -5.868      17.894      2.546      3.514      0.591      1745.40
48 5.000      -7.678      14.896      2.131      3.495      0.613      1771.52
49 5.100      -7.787      11.483      1.745      3.291      0.620      1701.26
50 5.200      -6.668      9.399      1.558      3.016      0.601      1589.64

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51	5.300	-5.654	8.308	1.482	2.802	0.577	1505.35
52	5.400	-4.915	7.717	1.455	2.652	0.554	1451.50
53	5.500	-4.528	7.308	1.426	2.562	0.542	1428.14
54	5.600	-4.280	6.832	1.375	2.484	0.534	1410.02
55	5.700	-3.924	6.317	1.325	2.383	0.522	1376.99
56	5.800	-3.509	5.924	1.299	2.280	0.504	1340.27
57	5.900	-3.073	5.680	1.301	2.183	0.483	1305.47
58	6.000	-2.681	5.644	1.336	2.113	0.461	1285.10
59	=h==	* indicate end of information					

6.6.12 W.IN_SB

1	-----						
2	Optical Properties of: Indium Antimonide (InSb)						
3							
4	D.E. Aspnes & A.A. Studna,						
5	Physical Review B, Volume 27, Number 2, 1983, January, 15.						
6	Pages: 985-1009.						
7							
8	-----						
9	E(eV),	<e1>,	<e2>,	n,	k,	R,	alpha*1.OE3 (cm**-1)
10	-----						
11	=h==	^ indicate end of header information					
12	46	^ quantity of lines of data					
13	1.500	19.105	5.683	4.418	0.643	0.406	97.79
14	1.600	20.302	6.838	4.568	0.749	0.421	121.39
15	1.700	21.699	9.019	4.754	0.949	0.441	163.46
16	1.800	22.148	13.707	4.909	1.396	0.467	254.73
17	1.900	16.144	16.603	4.433	1.873	0.463	360.65
18	2.000	14.448	14.875	4.194	1.773	0.443	359.46
19	2.100	13.974	14.643	4.136	1.770	0.439	376.79
20	2.200	13.674	15.302	4.135	1.850	0.445	412.62
21	2.300	12.653	16.936	4.111	2.060	0.458	480.25
22	2.400	9.377	17.480	3.822	2.287	0.463	556.30
23	2.500	7.811	15.856	3.570	2.221	0.447	562.77
24	2.600	7.278	14.787	3.447	2.145	0.434	565.33
25	2.700	7.069	14.069	3.377	2.083	0.425	570.01
26	2.800	7.044	13.617	3.345	2.036	0.419	577.71
27	2.900	7.150	13.395	3.342	2.004	0.415	589.12
28	3.000	7.354	13.421	3.366	1.994	0.416	606.27
29	3.100	7.627	13.779	3.419	2.015	0.420	633.20
30	3.200	7.742	14.572	3.482	2.093	0.431	678.77
31	3.300	7.507	15.631	3.525	2.217	0.445	741.69
32	3.400	6.782	16.678	3.520	2.369	0.459	816.31
33	3.500	5.995	17.673	3.511	2.517	0.474	892.82
34	3.600	4.830	18.854	3.485	2.705	0.492	987.01
35	3.700	3.147	20.102	3.427	2.933	0.514	1099.83
36	3.800	0.534	21.064	3.287	3.204	0.541	1234.25
37	3.900	-2.838	21.177	3.044	3.479	0.572	1375.21
38	4.000	-6.722	19.443	2.632	3.694	0.608	1497.79
39	4.100	-8.911	15.595	2.127	3.666	0.633	1523.33
40	4.200	-8.580	12.296	1.791	3.433	0.634	1461.59
41	4.300	-7.678	10.382	1.618	3.209	0.623	1398.45
42	4.400	-6.910	9.191	1.515	3.034	0.610	1353.08
43	4.500	-6.297	8.351	1.443	2.894	0.598	1320.24
44	4.600	-5.788	7.690	1.385	2.776	0.586	1294.36
45	4.700	-5.324	7.160	1.341	2.669	0.574	1271.51
46	4.800	-4.912	6.761	1.312	2.576	0.562	1253.17
47	4.900	-4.534	6.492	1.301	2.495	0.548	1239.36
48	5.000	-4.250	6.378	1.307	2.441	0.537	1237.01
49	5.100	-4.190	6.360	1.309	2.430	0.534	1255.97
50	5.200	-4.359	6.207	1.270	2.444	0.543	1288.04

51	5.300	-4.505	5.815	1.194	2.435	0.556	1308.25
52	5.400	-4.487	5.345	1.116	2.394	0.563	1310.58
53	5.500	-4.325	4.931	1.057	2.333	0.563	1300.55
54	5.600	-4.126	4.664	1.025	2.275	0.558	1291.44
55	5.700	-3.995	4.470	1.000	2.235	0.555	1291.22
56	5.800	-3.945	4.282	0.969	2.210	0.558	1299.21
57	5.900	-3.925	4.029	0.922	2.185	0.565	1306.73
58	6.000	-3.835	3.681	0.861	2.139	0.572	1300.85
59	=h==	" indicate end of information					

6.6.13 W.AL_SB

```

1 -----
2 Optical Properties of:      Aluminum Antimonide (AlSb)
3
4 S. Zollner, C. Lin, E. Schonherr, A. Bohringer, and M. Cardona
5 Journal of Applied Physics, Volume 66, Number 1, 1 July 1989.
6 Pages: 383-387.
7 -----
8 E(eV),      <e1>,      <e2>,      n,      k,      R,      alpha*1.0E3 (cm**-1)
9 -----
10 =h==              " indicate end of header information
11 45                " quantity of lines of data
12 1.400      12.23      0.0007      3.50      0.0001      0.308      0.02
13 1.500      12.56      0.001      3.54      0.0002      0.312      0.03
14 1.600      12.91      0.002      3.60      0.0003      0.319      0.05
15 1.700      13.30      0.007      3.66      0.001      0.325      0.2
16 1.800      13.93      0.015      3.73      0.002      0.333      0.3
17 1.900      14.53      0.02      3.81      0.003      0.341      0.6
18 2.000      15.24      0.03      3.90      0.004      0.350      0.8
19 2.100      16.08      0.05      4.01      0.006      0.361      1.3
20 2.200      17.54      0.08      4.20      0.01      0.378      2.4
21 2.300      18.50      2.11      4.31      0.24      0.390      57.1
22 2.400      19.62      2.99      4.44      0.33      0.402      82.0
23 2.500      20.97      4.25      4.61      0.46      0.417      117.0
24 2.600      22.76      6.09      4.81      0.63      0.436      166.8
25 2.700      24.98      9.35      5.08      0.92      0.462      252.1
26 2.800      25.30      16.70      5.27      1.58      0.496      449.3
27 2.900      17.41      19.19      4.66      2.06      0.486      605.7
28 3.000      16.54      17.82      4.52      1.97      0.473      599.0
29 3.100      16.30      19.43      4.57      2.12      0.485      668.0
30 3.200      14.24      22.35      4.51      2.47      0.505      803.1
31 3.300      9.91      22.32      4.14      2.69      0.508      900.8
32 3.400      8.77      21.00      3.97      2.64      0.498      911.2
33 3.500      8.31      21.33      3.95      2.69      0.503      957.7
34 3.600      7.72      22.32      3.96      2.81      0.513      1028.7
35 3.700      6.63      23.35      3.91      2.97      0.525      1113.8
36 3.800      4.53      24.12      3.81      3.16      0.540      1218.3
37 3.900      2.16      25.22      3.71      3.40      0.560      1345.0
38 4.000      -1.56      26.00      3.50      3.71      0.588      1506.1
39 4.100      -6.14      25.24      3.15      4.00      0.621      1665.6
40 4.200      -11.16      21.99      2.60      4.22      0.662      1799.7
41 4.300      -12.73      15.94      1.96      4.07      0.691      1776.3
42 4.400      -11.20      11.81      1.59      3.70      0.688      1653.6
43 4.500      -9.41      9.81      1.45      3.39      0.669      1547.4
44 4.600      -8.11      8.71      1.38      3.16      0.648      1475.0
45 4.700      -7.17      7.97      1.33      2.99      0.629      1425.2
46 4.800      -6.40      7.42      1.30      2.84      0.611      1384.6
47 4.900      -5.76      7.06      1.29      2.72      0.592      1354.9
48 5.000      -5.29      6.85      1.30      2.64      0.576      1338.8
49 5.100      -5.00      6.77      1.31      2.59      0.565      1339.4
50 5.200      -4.95      6.74      1.31      2.58      0.563      1360.3

```


51	5.300	-5.15	6.53	1.26	2.59	0.574	1394.7
52	5.400	-5.30	6.02	1.17	2.58	0.589	1413.2
53	5.500	-5.18	5.51	1.09	2.52	0.593	1407.9
54	5.600	-5.00	5.12	1.04	2.46	0.594	1399.9
55	5.700	-4.84	4.88	1.01	2.42	0.592	1398.7
56	5.800	-4.81	4.78	1.00	2.40	0.593	1415.3
57	=h==	* indicate end of information					

7. Acknowledgments

It is the author's pleasure to acknowledge Dr. George Candela for his suggestions and support during the course of this project. The author appreciates the questions and suggestions from Deane Chandler-Horowitz and Pradip Dutta, who have been among the first to apply the software package. Somewhere during the middle of the development of this software, the author had the expressed good fortune of receiving an invitation from Drs. Paul G. Snyder and John A. Woollam to attend a week-long seminar regarding ellipsometry that they were organizing at the University of Nebraska-Lincoln. The author appreciates the many fine presentations of and discussions with the staff and invited speakers, as well as the hospitality that was extended to all of the participants.

Regarding the database of dielectric functions for the constituent media, these were collected from the literature and serve so vitally in advancing various applications of spectroscopic ellipsometry. Such collections of data are products of much labor and incorporate much relevant physics. It would be a serious omission to fail to include special mention of appreciation of those who have made such databases available. Among them, the author especially appreciates the work reported by Dr. David E. Aspnes and associates.

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Appendix

Quick Reference Guide for NIST Special Publication 400-84

Semiconductor Measurement Technology:
**A Software Program for Aiding the
Analysis of Ellipsometric Measurements,
Simple Spectroscopic Models**

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National Institute of Standards and Technology
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1. Introduction

MAIN2 is a software program for analyzing spectroscopic ellipsometric measurements. The solid material sample is assumed to be nonmagnetic and to exhibit depth-dependent optical properties, such as one with layered structure atop a substrate, where the substrate behaves like a semi-infinite half-space, and where the layers are flat and of uniform thickness. The ambient region refers to that region of space that lies external to the layers-substrate region of the sample. The optical medium within each ambient/layer/substrate region is assumed to be isotropic, homogeneous, local, and linear. The dielectric function of an optical medium is represented by the Bruggeman effective medium approximation (EMA). An effective medium is represented as a mixture of distinct constituent bulk media, where the optical properties of each constituent medium is known a priori. The ellipsometric equations are solved for the model parameters by using a damped least-squares method.

The program involves at least five data files. These include: X.DAT, an input data file of the model parameters and measurement data; X.INN, an input data file of command options controlling the program; X.OUT, an output data file journaling the activity of the program; X.PLOT, an output data file of results suitable for later plotting; and W.*, the data files that contain the dispersion relationships of the distinct constituent media that are used in representing the effective media of the sample.

2. Input Data Requirements

The input data file X.DAT contains both the model parameters that characterize the layered structure of the sample and the ellipsometric measurement data. Each subsection presents a format convention that is used in forming the input file X.DAT for one particular subset of these input data. The subsections are presented in the order that the subsets are to appear in the input file. Each subset of entries is separated by a demarcation line that is made of connected hyphens and is at least 50 characters in length. Parameters that are shown to be capped with a tilde refer to index labels of array elements.

2.1 Database Information

The first line in file X.DAT specifies the location of the database files. The database files contain the optical properties or complex dielectric functions as functions of energy or optical frequency of the distinct constituent media. These constituent media are used in rep-

representing the effective media of the ambient/layers/substrate regions. The format convention for specifying the location of the database files is of the form:

$$\text{disk:}[\text{directory}]w.$$

where 'disk' refers to the name of the mass-storage device, 'directory' refers to the name of the directory that contains the database files of the constituent media, and 'w' is the filename of the various database files. The database file of a particular constituent medium has a distinct extension in its filename specification; the appropriate extension is supplied by the program.

2.2 Layer Thicknesses

The format convention for specifying the layer thicknesses is of the form:

$$m_z / (i, z_i, \delta z_i, v_i)$$

where:

m_z is the number of distinct thicknesses;

i is an integer that indexes the line entries consecutively in unit increments,
i.e., ($i = 1, 2, 3, \dots, m_z$);

z_i is the thickness of a layer measured in nanometers;

δz_i is the uncertainty that is assigned to the numerical value of z_i ; and

v_i is the integer (froz/vary) switch with value 0 or 1, respectively.

The forward slash mark '/' delimits the first line of input data. The parentheses bound items that ought to appear on each subsequent line of data until the implied DO-loop has been satisfied. Incidentally, if ($m_z = 0$), this is the only line of information that ought to be entered for this set of data, i.e., apart from the short line of connected hyphens for demarcation.

2.3 Supplementary Parameters (Integer)

The format convention for specifying the integer supplementary parameters is of the form:

$$m_I / (i, p_i)$$

where:

m_I is the number of distinct integer supplementary parameters;

i is an integer that indexes the line entries of data consecutively in unit increments, i.e., ($i = 1, 2, 3, \dots, m_I$); and

p_i is the integer supplementary parameter.

Since integer parameters are not subjected to optimization, no uncertainties are included regarding their numerical value.

2.4 Supplementary Parameters (Floating-Point)

The format convention for specifying the floating-point supplementary parameters is of the form:

$$m_R / (i, p_i, \delta p_i, v_i)$$

where:

m_R is the number of distinct floating-point supplementary parameters;

i is an integer that indexes the line entries of data consecutively in unit increments, i.e., ($i = 1, 2, 3, \dots, m_R$);

p_i is the floating-point supplementary parameter;

δp_i is the uncertainty that is assigned to the numerical value of p_i ; and

v_i is the integer (froz/vary) switch with value of either 0 or 1, respectively.

2.5 Effective Media or Mixtures

For each effective medium used in the ambient/layers/substrate regions, one must specify the constituent media and their volume fractions. The format convention for specifying the effective media or mixtures is of the form:

$$\begin{array}{c}
m_{\text{media}} \\
\vdots \\
m_{f,j}, m_{I,j}, m_{R,j} \quad / (i_f, \tilde{\epsilon}_i, f_i, \delta f_i, v_i) \\
\quad \quad \quad / (i_I, \tilde{p}_{I,i}) \\
\quad \quad \quad / (i_R, \tilde{p}_{R,i}) \\
\vdots
\end{array}$$

where:

m_{media} is the number of distinct effective media, i.e., ($m_{\text{media}} \geq 2$);

j is an integer that indexes the distinct effective media, i.e., ($j = 1, 2, \dots, m_{\text{media}}$);

$m_{f,j}$ is the number of distinct constituent media (or volume fractions) that are associated with the j^{th} effective medium;

$m_{I,j}$ is the number of integer supplementary parameters that are associated with the j^{th} effective medium;

$m_{R,j}$ is the number of floating-point supplementary parameters that are associated with the j^{th} effective medium;

i_f is an integer that locally indexes the distinct constituent media (or volume fractions) of the j^{th} effective medium, i.e., ($i_f = 1, 2, \dots, m_{f,j}$);

$\tilde{\epsilon}_i$ is an integer index label of the appropriate constituent medium that is associated with the i_f^{th} constituent medium of the j^{th} effective medium;

f_i is the volume fraction of the i_f^{th} constituent medium of the j^{th} effective medium;

δf_i is the uncertainty that is assigned to the numerical value of f_i ;

v_i is the integer (froz/vary) switch for f_i with value 0 or 1, respectively;

i_I is an integer that locally indexes the integer supplementary parameters that are associated with the j^{th} effective medium, i.e., ($i_I = 1, 2, \dots, m_{I,j}$);

$\tilde{p}_{I,i}$ is the integer index label of the appropriate integer supplementary parameter that is associated with the i_I^{th} integer supplementary parameter of the j^{th} effective medium, i.e., ($1 \leq \tilde{p}_{I,i} \leq m_I$);

i_R is an integer that locally indexes the floating-point supplementary parameters that are associated with the j^{th} effective medium, i.e., $(i_R = 1, 2, \dots, m_{R,j})$; and $\bar{p}_{R,i}$ is the integer index label of the appropriate floating-point supplementary parameter that is associated with the i_R^{th} floating-point supplementary parameter of the j^{th} effective medium, i.e., $(1 \leq \bar{p}_{R,i} \leq m_R)$.

2.6 Ambient and External Parameters

The ambient region refers to that spatial region that lies external to the layered structure of the sample. The indexed listing associates distinct effective media with distinct subsets of the supplementary parameters. The format convention for specifying the ambient and the external parameters is of the form:

$$\begin{array}{l} m_{\text{ambients}} \\ \vdots \\ j, \bar{e}_j, m_{I,j}, m_{R,j} \quad / (i_I, \bar{p}_{I,i}) \\ \quad \quad \quad \quad \quad \quad / (i_R, \bar{p}_{R,i}) \\ \vdots \end{array}$$

where:

m_{ambients} is the number of distinct ambients which involve associating effective media with subsets of the supplementary parameters;

j is an integer that indexes the distinct ambients, i.e., $(j = 1, 2, \dots, m_{\text{ambients}})$;

$\bar{e}_j$ is an integer index label of the appropriate effective (not constituent) medium that is associated with the j^{th} ambient, i.e., $(1 \leq \bar{e}_j \leq m_{\text{media}})$;

$m_{I,j}$ is the number of integer supplementary parameters that are associated with the j^{th} ambient;

$m_{R,j}$ is the number of floating-point supplementary parameters that are associated with the j^{th} ambient;

i_I is an integer that locally indexes the integer supplementary parameters that are associated with the j^{th} ambient, i.e., $(i_I = 1, 2, \dots, m_{I,j})$;

$\tilde{p}_{I,i}$ is the integer index label of the appropriate integer supplementary parameter that is associated with the i_I^{th} integer supplementary parameter of the j^{th} ambient, i.e., $(1 \leq \tilde{p}_{I,i} \leq m_I)$;

i_R is an integer that locally indexes the floating-point supplementary parameters that are associated with the j^{th} ambient, i.e., $(i_R = 1, 2, \dots, m_{R,j})$; and

$\tilde{p}_{R,i}$ is the integer index label of the appropriate floating-point supplementary parameter that is associated with the i_R^{th} floating-point supplementary parameter of the j^{th} ambient, i.e., $(1 \leq \tilde{p}_{R,i} \leq m_R)$.

2.7 Sample Characterization or Construction

The samples are constructed or assembled in a layer-by-layer fashion. Each spatial region requires an effective medium, and if the region is a layer, a thickness is required as well. Index labels are used to specify the configuration of the (layers/substrate) system. The format convention for specifying the layered structure of the samples is of the form:

$$\begin{array}{c}
 m_{\text{samples}} \\
 \vdots \\
 m_{z,j} \quad / \quad (i, \tilde{e}_i, \tilde{z}_i) \\
 \quad \quad \quad / \quad m_{z,j}+1, \tilde{e}_{\text{substrate},j} \\
 \vdots
 \end{array}$$

where:

m_{samples} is the number of distinct material samples being analyzed.

j is an integer that indexes the distinct samples, i.e., $(j = 1, 2, \dots, m_{\text{samples}})$.

$m_{z,j}$ is the number of layers that lie atop the substrate of the j^{th} sample.

i is an integer that locally indexes the distinct layers of the j^{th} sample, i.e., $(i = 1, 2, \dots, m_{z,j})$. The layer adjacent to the ambient is indexed 1, and the layer adjacent to the substrate is indexed $m_{z,j}$.

$\tilde{e}_i$ is the integer index label of the appropriate effective medium that is associated with the i^{th} layer of the j^{th} sample, i.e., $(1 \leq \tilde{e}_i \leq m_{\text{media}})$.

$\tilde{z}_i$ is the integer index label of the appropriate thickness that is associated with the i^{th} layer of the j^{th} sample, i.e., $(1 \leq \tilde{z}_i \leq m_z)$.

2.8 Measurement Data (Δ, ψ)

The measurement data of ellipsometric angles are organized in the same fashion that the samples are constructed, i.e., sample by sample. The data structure is of the form:

(angles & wavelengths, repeats, ambients, samples)

where:

samples indexes the set of distinct samples;

ambients indexes the set of distinct ambients involving a given sample;

repeats indexes the sets of distinct repeats of multiple-angle of incidence and multiple-optical frequency measurements of a system involving a given ambient and sample; and

angles & wavelengths indexes the set of distinct angles of incidence and optical frequencies (or wavelengths) used during the measurements of a system involving a given repeat index, ambient, and sample.

The measurement data are grouped sample by sample. For each sample, they are grouped ambient by ambient. For each ambient, they are grouped by their repeat index label. For each repeat index, they are indexed by both source variables, i.e., the angle of incidence and the optical frequency (or wavelength in vacuum or corresponding energy) of the light. The format convention for associating the measurement data with the sample, e.g., sample s , is of the form:

$$\begin{array}{c}
 m_{as} \\
 \vdots \\
 m_{ras} \quad \tilde{a}_s \\
 \vdots \\
 m_{\lambda\phi,ras} / (i, \lambda_i, \phi_i, \Delta_i, \psi_i / \delta\lambda_i, \delta\phi_i, \delta\Delta_i, \delta\psi_i)_{ras} \\
 \vdots \\
 \vdots
 \end{array}$$

where:

s is an integer that indexes the samples, i.e., $(s = 1, 2, \dots, m_{\text{samples}})$.

m_{as} is the number of ambients associated with sample s .

a_s is an integer that locally indexes the ambients associated with sample s , i.e., $(a_s = 1, 2, \dots, m_{as})$.

$\tilde{a}_s$ is the integer index label of the appropriate ambient that is associated with the a_s^{th} ambient on sample s .

m_{ras} is the number of sets of repeat measurements of (Δ, ψ) involving the a_s^{th} ambient on sample s .

$m_{\lambda\phi,ras}$ is the number of measurements of ellipsometric angles (Δ, ψ) involving multiple-angles of incidence and multiple-optical frequencies (or wavelengths in vacuum or associated energies) that involve the r_{as}^{th} repeat set of measurements, i.e., $(r_{as} = 1, 2, \dots, m_{ras})$, and the a_s^{th} ambient of sample s .

i is an integer that locally indexes the multiple-angle of incidence and multiple-optical frequency measurement data consecutively with unit increments, i.e., $(i = 1, 2, \dots, m_{\lambda\phi,ras})$.

λ_i is a floating-point source variable that may be of either sign depending upon how one chooses to characterize the optical frequency of light. When the value is negative, the unit of measure is nanometers. When the value is positive, the unit of measure is electron-volts. The program check-tests for either $(-1240 \leq \lambda_i \leq -200)$ or $(1.0 \leq \lambda_i \leq 6.0)$.

$\delta\lambda_i$ is the uncertainty that is assigned to the numerical value of λ_i .

ϕ_i is the angle of incidence measured in degrees, where a value of zero relates to that of normal incidence, i.e., $(0 \leq \phi_i \leq 90)$.

$\delta\phi_i$ is the uncertainty that is assigned to the numerical value of ϕ_i .

Δ_i is an ellipsometric angle measured in degrees, i.e., $(0 \leq \Delta_i < 360)$, assuming the engineering or Nebraska convention, i.e., $R_{p,H}$.

$\delta\Delta_i$ is the uncertainty that is assigned to the numerical value of Δ_i .

ψ_i is an ellipsometric angle measured in degrees, i.e., ($0 \leq \psi_i \leq 90$).

$\delta\psi_i$ is the uncertainty that is assigned to the numerical value of ψ_i .

Within any set of $m_{\lambda\phi,ras}$ measurement data, ordering among the angles of incidence or among the optical frequencies (or wavelengths in vacuum or associated energies) is not necessarily important.

To construct the final set of data that includes all of the samples, one simply concatenates the data of the individual samples together, i.e., without any intervening lines of demarcation.

3. Command Options

The input data file X.INN contains the list of command options that direct the control of the software package. To direct the execution of the program, a menu-driven decision tree of command options is made available to the user. The subsections are presented in the order that the options are listed at level one. The first level of the tree involves a menu of three options.

```
Enter:  option
        1, forward problems, plots, ...
        2, search      (vary)
        3, search grid (vary)
```

where the options at level one include:

- 1, requests the program to perform one of several simple tasks, such as providing a set of tabulated output that is amenable for plotting or initiating a series of calculations of the direct or forward problem. No iterative calculations are considered, i.e., no minimizations or inversions of the ellipsometric equations.
- 2, requests the program to invert the ellipsometric equations by performing a series of unconstrained optimization calculations.
- 3, requests the program to invert the ellipsometric equations by performing a grid scan over a selected set of model parameters. A series of constrained optimization calculations is initiated at each point of the grid of model parameters.

3.1 Forward Problems, Plots, ...

This option provides simulations of the forward problem, i.e., option '1' at level one. The next set of options requests the type of grid used for the source variables (λ, ϕ), i.e., the optical frequency (or wavelength in vacuum or corresponding energy) and the angle of incidence. The menu of options at level two is:

```
Enter:  choice of incident (energies, angles)
        1,  measurement data,      x.dat
        2,  grid scan.
```

where the options at level two involve:

- 1, requests the program to use as source variables only those sets of ordered pairs (λ, ϕ) that are specified in the input file X.DAT for the measurement data of (Δ, ψ).
- 2, requests the program to use as source variables only those sets of ordered pairs (λ, ϕ) that lie on a two-dimensional grid that is specified later in a following prompt-request. The program prompts or requests information regarding the lower bound, the upper bound, and the stepsize for each dimension of the grid.

The next step in the program involves specifying which field quantities are to be calculated and written to the output file X.PLOT. Two alternative sets of options are presented in succession.

Following the selection of option '1' at level two, the menu of options at level three is:

```
Enter:  choice of output suitable for:
        1,  input data,      x.dat,
        2,  plotting (Delta, psi),
        3,  plotting (Delta, psi) deviations,
            deviation = measurement - model.
        4,  plotting |g| ~ rms deviation,  unscaled,
            on a 1D or 2D grid of model parameters.
```

where:

- 1, requests the program to calculate (Δ, ψ) using (λ, ϕ) as supplied by the file X.DAT. The output is written to the plot file X.PLOT. The format is suitable for use in file X.DAT.

- 2, requests the program to calculate (Δ, ψ) using (λ, ϕ) as supplied by the file X.DAT. The output is written to the plot file X.PLOT. The format is suitable for later graphics.
- 3, requests the program to calculate and tabulate the deviations between the measurement data and that calculated by the model. The output is written to the plot file X.PLOT.
- 4, requests the program to initiate a grid scan of model parameters and evaluate the error expression $|g|$ for each point on the grid. For convenience, the grid may be either one or two dimensional; i.e., only one or two model parameters may undergo variation. To specify the grid of 'vary' model parameters, see section 3.3, but note that there is no option regarding optimization here. The output is written to file X.PLOT.

Alternatively, following the selection of option '2' at level two, the menu of options at level three is:

```

Enter:  choice of output suitable for:
        1,  dielectric function,  media,
        2,  (Delta, psi),          x.dat,
        3,  (Delta, psi),          plotting,
        4,  d/db,                  b'(z,f,p),
        5,  d/da,                  angle of incidence,
        6,  d/dE,                  energy.

```

where:

- 1, requests the program to calculate the dielectric function for an effective medium that is specified later. The format is suitable for later graphics.
- 2, requests the program to calculate (Δ, ψ) for a grid of (λ, ϕ) . The format is suitable for use in file X.DAT.
- 3, requests the program to calculate (Δ, ψ) for a grid of (λ, ϕ) . The format is suitable for later graphics.
- 4, requests the program to calculate partial derivatives of (Δ, ψ) with respect to one of the model parameters, i.e., thickness, volume fraction, or supplementary parameter. Since volume fractions involve a linear constraint, the partial derivative with

respect to $\hat{f}_j$ is calculated according to eq (10), where ($k < j$). Again, if the selection involves volume fractions, two volume fractions must be selected to undergo variation; that which is associated with $\hat{f}_j$, as given by eq (10), is written to the file X.PLOT. The model parameter is selected by setting the (froz/vary) switch to '1' in X.DAT. The unit of measure is degree per unit of the 'vary' model parameter.

5, requests the program to calculate partial derivatives of (Δ, ψ) with respect to the angle of incidence, ϕ . The measure is unitless, i.e., degree per degree.

6, requests the program to calculate partial derivatives of (Δ, ψ) with respect to the corresponding energy of light. The unit measure is degree per electron-volt.

If the dielectric function of option '1' is selected from the above list, then the associated effective medium must be specified next.

```
Enter:   kmix " effective medium of dielectric function
```

where 'kmix' is the integer index label of the particular effective medium.

Finally, regarding the grid of source variables (λ, ϕ), the grid is established by specifying for each axis of the grid the lower bound, the upper bound, and the stepsize.

The first axis involves the grid of optical frequencies, wavelengths in vacuum, or associated energies.

```
Enter:   range of incident energies (eV)
         or:                - wavelengths (nm)
Enter:   ev1, ev2, ev3
```

where ev1 is the lower bound, ev2 is the upper bound, and ev3 is the stepsize. Negative values are associated with wavelength in units of nanometers, and positive values are associated with frequency as expressed by energy in units of electron-volts.

The second axis involves the grid of angles of incidence.

```
Enter:   range of incident angles (degrees)
Enter:   angle1, angle2, angle3
```


where *angle1* is the lower bound, *angle2* is the upper bound, and *angle3* is the stepsize. Numerical values are positive and are in units of degrees.

3.2 Search (vary)

This option lets the program invert the ellipsometric equations by minimizing the error expression as an unconstrained optimization problem, i.e., option '2' at level one. No further options are required here. At least one model parameter must be set to undergo variation in file X.DAT for each set of measurement data being analyzed. Regarding the 'vary' model parameters, the stepsizes of the Newton steps are scaled by the numerical values of the uncertainties.

3.3 Search Grid (vary)

This option lets the program invert the ellipsometric equations by minimizing the error expression as a constrained optimization problem, i.e., option '3' at level one. This involves scanning a grid of model parameters; the grid is scanned from a set of nested DO-loops; the grid is established as a direct product of its axes. Each axis involves one distinct model parameter and is characterized by its lower bound, upper bound, and stepsize. The program issues the following prompt-request:

```
Scan a grid of model parameters: (z,p,f).  
Grid info: DO-loop parameters  
Grid info: i, initial, final, increment.
```

For each model parameter selected to undergo variation, the format convention for specifying the range of the DO-loop to characterize the axis of the grid is of the form:

$$i_p, p_1, p_2, p_3,$$

where i_p refers to the local integer index label of the model parameter p , and p_j refers to the numerical value of the model parameter that is associated with the initial value, final value, and stepsize, as appropriate. The model parameters are entered in the order of their placement in the input file X.DAT. Regarding the grid of volume fractions for a given effective medium, the grid specification skips the one with the smallest index label.

For each point of the multidimensional grid of model parameters, the program evaluates the error expression $|g|$. The program may then move to the next grid point, i.e., no optimization, or else use Newton steps to minimize $|g|$, i.e., full optimization. Accordingly, the program prompts the following list of options:

```
Enter:  option  regarding the grid scan:
        0,      no optimization, |g| only,
        1,      full optimization, Jacobian.
```

The format convention for indicating the type of optimization is of the form:

$$i_o$$

where i_o is an integer with value 0 or 1, accordingly.

4. Constituent Media

The effective medium of a ambient/layer/substrate region is modeled as a mixture composed of distinct constituent media. A constituent medium is characterized by its optical properties, i.e., complex dielectric function as a function of optical frequency. These dielectric functions of the constituent media are known a priori, and serve as basis functions in expressing the effective media. The following is the current indexed listing of constituent media.

- 1) vacuum
- 2) air
- 3) Si (crystalline)
- 4) Si (amorphous)
- 5) SiO₂ (amorphous)
- 6) Si₃N₄ (noncrystalline)
- 7) Ge (crystalline)
- 8) GaAs (crystalline)
- 9) Al_xGa_{1-x}As (crystalline)

- 10) Oxides of GaAs (amorphous)
- 11) As (amorphous)
- 12) GaP (crystalline)
- 13) GaSb (crystalline)
- 14) InAs (crystalline)
- 15) InP (crystalline)
- 16) InSb (crystalline)
- 17) AlSb (crystalline)

5. Example, SiO₂ on Si

This section presents an example of input files, X.DAT and X.INN, for a case of modeling a flat sample of silicon with a thermally grown oxide layer. For convenience, let the layered structure of the sample involve two layers and a substrate. Let the top layer be amorphous SiO₂ and be 100 nm thick; let the transition region be a 50-50 mixture of amorphous SiO₂ and crystalline Si and be 2 nm thick, and let the substrate be crystalline Si. An example of the input file X.DAT is the following:

```

1 drbl:[data_bases]w.
2 -----
3 2                      ! mfilmz " thicknesses /(i,z,zu,ivary)
4 1    100.0    2.0    0    ! i,z,zu,ivary " top layer, SiO2
5 2      2.0    2.0    1    ! i,z,zu,ivary " bottom layer, SiO2+Si
6 -----
7 0                      ! mipars / (i,ip)
8 -----
9 0                      ! mrpars / (i,rp,up,ivary)
10 -----
11 4                      ! mixtures " number of effective media
12 1 0 0                  ! mlmnt,mipar,mrpar #1
13 1 2 1.0 0.0 0          ! j,lmnt,frac,ufrac,ivary " air
14 1 0 0                  ! mlmnt,mipar,mrpar #2
15 1 3 1.0 0.0 0          ! j,lmnt,frac,ufrac,ivary " Si
16 1 0 0                  ! mlmnt,mipar,mrpar #3
17 1 5 1.0 0.0 0          ! j,lmnt,frac,ufrac,ivary " SiO2
18 2 0 0                  ! mlmnt,mipar,mrpar #4
19 1 3 0.5 0.02 1         ! j,lmnt,frac,ufrac,ivary " Si
20 2 5 0.5 0.02 1         ! j,lmnt,frac,ufrac,ivary " SiO2

```

```

21 -----
22 1                      ! mbient " number of ambients
23      1 1 0 0          ! j,imix,mipar,mrpar      " air
24 -----
25 1                      ! msampl " number of samples analyzed
26 2                      ! mfilm " number of layers on sample #1
27      1 3 1            ! j,imix,iz      " SiO2      , top layer
28      2 4 2            ! j,imix,iz      " SiO2+Si, transition region
29      3 2              ! j,imix        " Si        , substrate
30 -----
31 1                      ! mbien " number of ambients on sample #1
32 1 1                    ! mrpeat,imbien
33 10                     ! mexpt " number of measurements
34 1      1.50000E+00 7.00000E+01 8.04309E+01 3.08875E+01 (i,E,a, d,p)
35      1.00000E-01 1.00000E-02 1.00000E-02 1.00000E-02 (uncertainty)
36 2      2.00000E+00 7.00000E+01 7.97129E+01 4.31275E+01 (i,E,a, d,p)
37      1.00000E-01 1.00000E-02 1.00000E-02 1.00000E-02 (uncertainty)
38 3      2.50000E+00 7.00000E+01 1.02227E+02 6.93018E+01 (i,E,a, d,p)
39      1.00000E-01 1.00000E-02 1.00000E-02 1.00000E-02 (uncertainty)
40 4      3.00000E+00 7.00000E+01 2.50415E+02 6.09989E+01 (i,E,a, d,p)
41      1.00000E-01 1.00000E-02 1.00000E-02 1.00000E-02 (uncertainty)
42 5      3.50000E+00 7.00000E+01 2.62427E+02 4.00376E+01 (i,E,a, d,p)
43      1.00000E-01 1.00000E-02 1.00000E-02 1.00000E-02 (uncertainty)
44 6      4.00000E+00 7.00000E+01 2.47313E+02 3.31054E+01 (i,E,a, d,p)
45      1.00000E-01 1.00000E-02 1.00000E-02 1.00000E-02 (uncertainty)
46 7      4.50000E+00 7.00000E+01 1.92800E+02 3.34557E+01 (i,E,a, d,p)
47      1.00000E-01 1.00000E-02 1.00000E-02 1.00000E-02 (uncertainty)
48 8      5.00000E+00 7.00000E+01 1.24499E+02 3.21867E+01 (i,E,a, d,p)
49      1.00000E-01 1.00000E-02 1.00000E-02 1.00000E-02 (uncertainty)
50 9      5.50000E+00 7.00000E+01 8.77637E+01 3.66717E+01 (i,E,a, d,p)
51      1.00000E-01 1.00000E-02 1.00000E-02 1.00000E-02 (uncertainty)
52 10     6.00000E+00 7.00000E+01 7.10687E+01 4.18238E+01 (i,E,a, d,p)
53      1.00000E-01 1.00000E-02 1.00000E-02 1.00000E-02 (uncertainty)

```

where the lines have been indexed or numbered for convenience and readability; the input file should *not* contain such indexing.

Line 1 specifies the location of the database files for the constituent media. Lines 3 to 5 refer to the distinct layer thicknesses. Line 7 refers to the integer supplementary parameters. Line 9 refers to the floating-point supplementary parameters. Lines 11 to 20 specify the effective media in terms of the constituent media. Lines 22 and 23 refer to the ambient and external parameters. Lines 25 to 29 specify the layered structure of the sample. Lines 31 to 53 refer to the collected set of simulated measurement data.

This example shows that three model parameters are selected to undergo variation, a thickness and two volume fractions; see lines 5, 19, and 20, respectively; the (froz/vary) switches are set to '1.' Hence, their numerical values will undergo variation if so requested from the

command options in file X.INN. These three model parameters are associated with the transition region; see line 28.

Regarding the selection of command options in input file X.INN, suppose now that a grid search is to be used to find the *best* solution for this set of vary model parameters. For convenience, let the thickness range from 1.0 to 3.0 nm in steps of 2.0 nm. Regarding volume fractions (f_i), the volume fraction with the smallest index label value of the effective medium is *not* entered in the specification of the grid. From lines 19 and 20, note that the volume fraction for crystalline silicon (f_{Si}) is listed *before* the volume fraction for amorphous SiO_2 (f_{SiO_2}); thus no grid information is entered for f_{Si} . Let f_{SiO_2} range from 0.3 to 0.7 in steps of 0.4. Lastly, let the grid search use Newton steps in the calculations. The input file X.INN would then be as follows:

```

3          ! search grid
2    1.0    3.0    2.0    ! thickness          transition region
2    0.3    0.7    0.4    ! volume fraction, oxide, transition region
1          ! full optimization, use the Jacobian

```

The output file X.OUT journals the activity of the program. The output file X.PLOT would contain the deviations between the measurement and the model.

6. Example, $Al_xGa_{1-x}As$ on GaAs

This section presents an example of using the supplementary parameters. Consider a flat sample of GaAs with a layer of $Al_xGa_{1-x}As$. Let the layered structure involve only the layer and the substrate. Let the layer be 50 nm thick, and let ($x = 0.3$) specify the mole fraction of aluminum. An example of the input file X.DAT is the following:

```

1  drb1:[data_bases]w.
2  -----
3  1          ! mfilmz / (j,z,zu,ivary)
4    1    50.    1.0    1    ! thickness, top layer
5  -----
6  1          ! mipars / (i,ip)
7    1    9          ! lmnt = 9, constituent = AlGaAs
8  -----
9  1          ! mrpars / (i,rp,up,ivary)
10   1    0.3    0.01    1    ! stoichiometry = x, Al(x)Ga(1-x)As
11  -----
12  3          ! mixtures = number of effective media
13  1    0    0    ! mlmnt,mipar,mrpar #1

```

```

14      1 2 1.0 0.0 0      !      j,lmnt,frac,ufrac,ivary  " air
15      1 0 0      !      mlmnt,mipar,mrpar      #2
16      1 8 1.0 0.0 0      !      j,lmnt,frac,ufrac,ivary  " GaAs
17      1 1 1      !      mlmnt,mipar,mrpar      #3
18      1 9 1.0 0.0 0      !      j,lmnt,frac,ufrac,ivary  " AlGaAs
19      1 1      !      i, iip
20      1 1      !      i, irp
21  -----
22      1      !      mbient " number of distinct ambients
23      1 1 0 0      !      j,imix,mipar,mrpar      " air
24  -----
25      1      !      msampl " number of samples
26      1      !      mfilm " number of layers on sample #1
27      1 3 1      !      j,imix,iz      " AlGaAs
28      2 2      !      j,imix      " GaAs substrate
29  -----
30      1      !      mbien " number of ambients for sample #1
31      1 1      !      mrpeat,imbien
32      12      !      mexpt " number of measurements
33      1 1.50000E+00 6.50000E+01 1.76446E+02 1.24387E+01 (i,E,a, d,p)
34      1.00000E-01 1.00000E-02 1.00000E-02 1.00000E-02 (uncertainty)
35      2 2.00000E+00 6.50000E+01 1.79401E+02 1.57825E+01 (i,E,a, d,p)
36      1.00000E-01 1.00000E-02 1.00000E-02 1.00000E-02 (uncertainty)
37      3 2.50000E+00 6.50000E+01 1.77396E+02 1.95307E+01 (i,E,a, d,p)
38      1.00000E-01 1.00000E-02 1.00000E-02 1.00000E-02 (uncertainty)
39      4 3.00000E+00 6.50000E+01 1.66208E+02 2.33677E+01 (i,E,a, d,p)
40      1.00000E-01 1.00000E-02 1.00000E-02 1.00000E-02 (uncertainty)
41      5 3.50000E+00 6.50000E+01 1.49379E+02 2.43128E+01 (i,E,a, d,p)
42      1.00000E-01 1.00000E-02 1.00000E-02 1.00000E-02 (uncertainty)
43      6 4.00000E+00 6.50000E+01 1.48705E+02 2.35367E+01 (i,E,a, d,p)
44      1.00000E-01 1.00000E-02 1.00000E-02 1.00000E-02 (uncertainty)
45      7 1.50000E+00 7.00000E+01 1.69646E+02 4.65575E+00 (i,E,a, d,p)
46      1.00000E-01 1.00000E-02 1.00000E-02 1.00000E-02 (uncertainty)
47      8 2.00000E+00 7.00000E+01 1.78701E+02 8.31343E+00 (i,E,a, d,p)
48      1.00000E-01 1.00000E-02 1.00000E-02 1.00000E-02 (uncertainty)
49      9 2.50000E+00 7.00000E+01 1.75534E+02 1.26304E+01 (i,E,a, d,p)
50      1.00000E-01 1.00000E-02 1.00000E-02 1.00000E-02 (uncertainty)
51      10 3.00000E+00 7.00000E+01 1.58723E+02 1.75083E+01 (i,E,a, d,p)
52      1.00000E-01 1.00000E-02 1.00000E-02 1.00000E-02 (uncertainty)
53      11 3.50000E+00 7.00000E+01 1.35016E+02 1.96919E+01 (i,E,a, d,p)
54      1.00000E-01 1.00000E-02 1.00000E-02 1.00000E-02 (uncertainty)
55      12 4.00000E+00 7.00000E+01 1.33538E+02 1.88574E+01 (i,E,a, d,p)
56      1.00000E-01 1.00000E-02 1.00000E-02 1.00000E-02 (uncertainty)

```

where the lines have been indexed for convenience and readability; the input file should not contain such indexing.

Lines 3 and 4 refer to the thickness of the layer. Lines 6 and 7 refer to the integer supplementary parameters; the integer parameter is used to specify a distinct constituent medium. Lines 9 and 10 refer to the floating-point supplementary parameters; the floating-

point parameter is used to specify the mole fraction of aluminum. Lines 19 and 20 are used to provide the necessary correspondence between the effective medium and the supplementary parameters. Two model parameters are shown to be selected for optimization, the layer thickness and the mole fraction of aluminum; two (froz/vary) switches are set to one; see lines 4 and 10. Lines 30 to 56 refer to simulated measurement data.

Regarding command options, suppose that a grid search is used to find the *best* solution. Let the thickness range from 40 to 60 nm in steps of 2 nm. Let the aluminum mole fraction range from 0.2 to 0.4 in steps of 0.02. Since the axes of the grid are specified according to the order that the model parameters are presented in the input file X.DAT, the specification for layer thickness precedes that for the mole fraction of aluminum; see lines 4 and 10 of file X.DAT. Let the grid search evaluate $|g|$ only at the grid points, i.e., no Newton steps. The input file X.INN would be as follows:

```

3          ! search grid
1  40.0    60.0    2.0    ! thickness, top layer, Al(x)Ga(1-x)As
1   0.2     0.4    0.02   ! stoichiometry,    x = Al
0                                     ! no optimization, grid points only

```


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☐ DOCUMENT DESCRIBES A COMPUTER PROGRAM; SF-185, FIPS SOFTWARE SUMMARY, IS ATTACHED.											
11. ABSTRACT (A 200-WORD OR LESS FACTUAL SUMMARY OF MOST SIGNIFICANT INFORMATION. IF DOCUMENT INCLUDES A SIGNIFICANT BIBLIOGRAPHY OR LITERATURE SURVEY, MENTION IT HERE.) MAIN2 is a software program for analyzing spectroscopic ellipsometric measurements. MAIN2 consists mainly of subroutines written in FORTRAN that are used to invert the standard reflection ellipsometry equations for simple systems. Here, a system is said to be simple if the solid material sample is characterized by models which assume at least the following: (1) materials are nonmagnetic; (2) samples exhibit depth-dependent optical properties, such as one with layered or laminar structure atop a substrate that behaves like a semi-infinite half-space; (3) layers are flat and of uniform thickness; and (4) the optical medium within each ambient/layer/substrate is isotropic, homogeneous, local, and linear. The ambient region refers to that region of space which lies external to the layer/substrate structure of the sample. Usually, the ambient region involves a medium of air or vacuum. Each layer is characterized by a thickness and a dielectric function. The dielectric function of a region, i.e., ambient, layer, or substrate, is represented by the Bruggeman effective medium approximation (EMA). Within the EMA, the effective medium of a region is characterized by an aggregate mixture of constituent media, and the dielectric function of each constituent medium is known a priori. The constituent dielectric functions are taken from the literature. The ellipsometric equations are formulated as a standard damped nonlinear least-squares problem and then solved by an iterative method when possible. The program is sufficiently modular to allow one to modify some of the models used in the calculations.											
12. KEY WORDS (6 TO 12 ENTRIES; ALPHABETICAL ORDER; CAPITALIZE ONLY PROPER NAMES; AND SEPARATE KEY WORDS BY SEMICOLONS) ellipsometry; EMA; FORTRAN; modeling; software; spectroscopic models											
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