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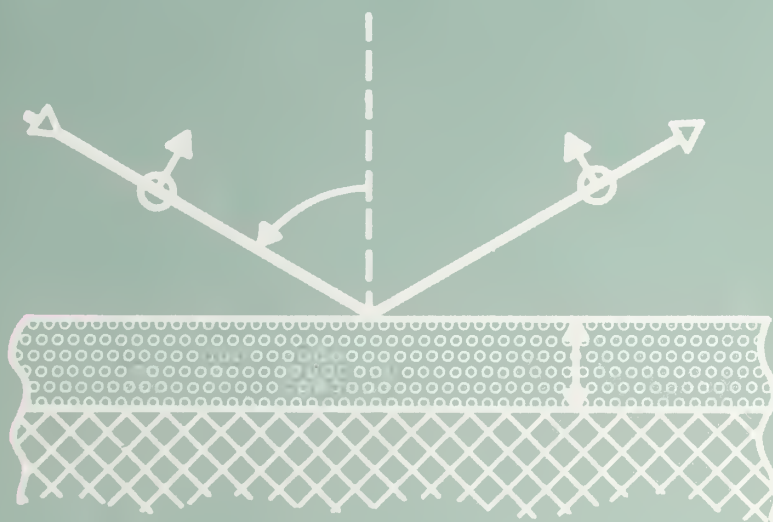
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U.S. DEPARTMENT OF COMMERCE/National Bureau of Standards

*Semiconductor Measurement Technology:***Analytic Analysis of
Ellipsometric Errors**

$$\begin{array}{ccc} \psi \pm \delta\psi, \Delta \pm \delta\Delta & \xrightarrow{\text{EEA}} & t \pm \delta t \\ \phi \pm \delta\phi, n_s \pm \delta n_s & & n_f \pm \delta n_f \end{array}$$

Deane Chandler-Horowitz

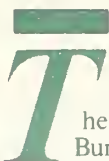
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Semiconductor Measurement Technology:

Analytic Analysis of Ellipsometric Errors

Deane Chandler-Horowitz

Semiconductor Electronics Division
Center for Electronics and Electrical Engineering
National Engineering Laboratory
Gaithersburg, MD 20899



U.S. DEPARTMENT OF COMMERCE, Malcolm Baldrige, Secretary

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Deane Chandler-Horowitz
Semiconductor Electronics Division
National Bureau of Standards
Gaithersburg, MD 20899

Abstract

A computer program is given that contains an explicit error analysis (EEA) for ellipsometric measurements. The program can identify the ellipsometric inaccuracies for any ellipsometer, can be used to determine which parameters contribute the most to the overall measurement inaccuracy, and can lead one to an optimum measurement procedure. A FORTRAN program that performs the evaluation of the partial derivative expressions needed to analyze ellipsometric measurement uncertainties is listed. The program determines the uncertainty in the calculation of the refractive index of a bare isotropic substrate or the uncertainty in the determination of the thickness and refractive index of a nonabsorbing film on a substrate of known refractive index. These are the two most commonly used surface models used in ellipsometry performed at single angle of incidence and a single wavelength. The program input parameters include the wavelength of light, the angle of incidence and its uncertainty, and the uncertainties in the ellipsometric parameters Δ and ψ . They also include in the ambient-substrate model an estimated value for the substrate's refractive index, and in the film-substrate model the refractive index of the substrate and its uncertainty and estimated values for the film's refractive index and thickness. The case of the conventional null ellipsometer utilizing a quarter-wave plate is treated to find the uncertainties in Δ and ψ from the uncertainties in the polarizer and analyzer null values and the waveplate constants.

Key words: bare substrate model; computer program; ellipsometric error analysis; film refractive index; film-substrate model; film thickness; substrate refractive index.

Introduction

A FORTRAN program was developed that calculates the ellipsometric measurement uncertainties for two models of a surface. The first is the simple bare isotropic substrate model. The second is the isotropic nonabsorbing film-substrate model. It is assumed that the sample to be measured ellipsometrically can be best described by one of these two models. From the ellipsometer, one obtains values for the two angular quantities Δ and ψ . These allow a determination of at least two of the unknown optical properties of the sur-

face. This corresponds to a determination of the real and imaginary parts of the substrate refractive index for the bare substrate model and a determination of the film's refractive index and thickness for the film-substrate model. In each case, a calculation involving the inversion of the ellipsometric equations is performed to solve for the unknown optical properties [1].

For an ideal ellipsometer, Δ and ψ are functions of up to six independent parameters: the ambient refractive index, the substrate refractive index, the film refractive index and thickness, the angle of incidence, and the wavelength. The measured or assumed values of these parameters may have systematic errors in addition to random errors. In an actual ellipsometer, the measured values of Δ and ψ are susceptible to other sources of errors. These can include azimuthal-angle errors, component and cell-window optical imperfections, beam deviation errors, parasitic beams, source-beam polarization and collimation errors, polarization-dependent detector sensitivity, and residual mechanical imperfections. Therefore, the ultimate accuracy for a nonideal ellipsometer can be limited by these other errors, and, for a further error investigation, one should assess the above errors. In the case of the conventional null instrument, the method of measuring Δ and ψ using four-zone averaging best ensures that Δ and ψ are free from most above cited imperfections [2]. The analytic functions for Δ and ψ can then be solved for the two unknown differentials that lead to a calculation of the uncertainty in the ellipsometrically measured quantities[3,4].

Theory and Calculations

The ellipsometric parameters Δ and ψ are defined by the complex reflectance ratio ρ as follows [5]:

$$\rho = \frac{R_p}{R_s} = \tan\psi e^{i\Delta}. \quad (1)$$

Here, R_p and R_s are the ratios of the reflected to the incident electric field amplitudes of the light for polarization parallel, p , and perpendicular, s , to the plane of incidence. In the case of light reflection from the ambient-substrate surface, the complex reflectances are:

$$R_p = \frac{n_s \cos\phi - n_0 \sqrt{1 - \left[\frac{n_0 \sin\phi}{n_s} \right]^2}}{n_s \cos\phi + n_0 \sqrt{1 - \left[\frac{n_0 \sin\phi}{n_s} \right]^2}} \quad (2)$$

$$R_s = \frac{n_0 \cos\phi - n_s \sqrt{1 - \left[\frac{n_0 \sin\phi}{n_s} \right]^2}}{n_0 \cos\phi + n_s \sqrt{1 - \left[\frac{n_0 \sin\phi}{n_s} \right]^2}}. \quad (3)$$

In the case of the ambient-film-substrate model, the reflectances are:

$$R_p = \frac{r_{p0f} + r_{pfs} e^{-i2\beta}}{1 + r_{p0f} r_{pfs} e^{-i2\beta}} \quad (4)$$

$$R_s = \frac{r_{s0f} + r_{sfs} e^{-i2\beta}}{1 + r_{s0f} r_{sfs} e^{-i2\beta}}, \quad (5)$$

where

$$r_{p0f} = \frac{n_f \cos\phi - n_0 \sqrt{1 - \left[\frac{n_0 \sin\phi}{n_f}\right]^2}}{n_f \cos\phi + n_0 \sqrt{1 - \left[\frac{n_0 \sin\phi}{n_f}\right]^2}} \quad (6)$$

$$r_{s0f} = \frac{n_0 \cos\phi - n_f \sqrt{1 - \left[\frac{n_0 \sin\phi}{n_f}\right]^2}}{n_0 \cos\phi + n_f \sqrt{1 - \left[\frac{n_0 \sin\phi}{n_f}\right]^2}} \quad (7)$$

$$r_{pfs} = \frac{n_s \sqrt{1 - \left[\frac{n_0 \sin\phi}{n_f}\right]^2} - n_f \sqrt{1 - \left[\frac{n_0 \sin\phi}{n_s}\right]^2}}{n_s \sqrt{1 + \left[\frac{n_0 \sin\phi}{n_f}\right]^2} + n_f \sqrt{1 - \left[\frac{n_0 \sin\phi}{n_s}\right]^2}} \quad (8)$$

$$r_{sfs} = \frac{n_f \sqrt{1 - \left[\frac{n_0 \sin\phi}{n_f}\right]^2} - n_s \sqrt{1 - \left[\frac{n_0 \sin\phi}{n_s}\right]^2}}{n_f \sqrt{1 + \left[\frac{n_0 \sin\phi}{n_f}\right]^2} + n_s \sqrt{1 - \left[\frac{n_0 \sin\phi}{n_s}\right]^2}}. \quad (9)$$

r_{p0f} and r_{s0f} are the real Fresnel reflection coefficients for the p and s polarizations of the electric field for the air-film interface. r_{pfs} and r_{sfs} are the corresponding complex Fresnel coefficients for the film-substrate interface. The refractive indices are n_0 for the ambient, n_f for the film, and n_s for the substrate. The angle of incidence is ϕ and the film phase thickness β is given in terms of the wavelength, λ , and film thickness, t , as follows:

$$\beta = \frac{2\pi t n_f}{\lambda} \sqrt{1 - \left[\frac{n_0 \sin\phi}{n_f}\right]^2}. \quad (10)$$

It should be noted that there is no explicit dependence on wavelength for the bare substrate model case.

The measurement uncertainties are derived for the bare substrate model as follows. The function ρ as given by eq (1) is a function of n_0 , n_s , and ϕ :

$$\rho = \rho(n_0, n_s, \phi). \quad (11)$$

The substrate's refractive index has, in general, a real and imaginary part:

$$n_s = n_{sr} - i n_{si}. \quad (12)$$

n_{sr} is the real part of the index of refraction, and n_{si} is the imaginary part, normally expressed as the extinction coefficient k .

By taking the total differential of eq (11), $d\rho$, and assuming the differential quantities $d\Delta$, $d\psi$, dn_0 , $d\phi$ correspond to experimentally known uncertainties, the following result for the uncertainty of n_s is obtained, neglecting the variation in n_0 :

$$dn_s = \frac{d\rho - \frac{\partial \rho}{\partial \phi} d\phi}{\frac{\partial \rho}{\partial n_s}}. \quad (13)$$

By eq (1), this expands to

$$dn_s = \frac{i \rho d\Delta + \sec^2 \psi e^{i\Delta} d\psi - \frac{\partial \rho}{\partial \phi} d\phi}{\frac{\partial \rho}{\partial n_s}}. \quad (14)$$

From eqs (1), (2), and (3),

$$\frac{\partial \rho}{\partial n_s} = - \frac{n_s (1 + \rho)^3 \cos^2 \phi}{2 (1 - \rho) n_0^2 \sin^4 \phi} \quad (15)$$

and

$$\frac{\partial \rho}{\partial \phi} = - \frac{\frac{\partial \rho}{\partial n_s} [n_s^2 (1 + \sec^2 \phi) + n_0^2 (1 - \sec^2 \phi)]}{n_s \tan \phi}. \quad (16)$$

Therefore,

$$dn_s = a_1 d\phi + a_2 d\Delta + a_3 d\psi, \quad (17)$$

where

$$a_1 = \frac{[n_s^2 (1 + \sec^2 \phi) + n_0^2 (1 - \sec^2 \phi)]}{n_s \tan \phi} \quad (18)$$

$$a_2 = 2 i \rho \frac{\rho - 1}{n_s (1 + \rho)^3} n_0^2 \sin^2 \phi \tan^2 \phi \quad (19)$$

$$a_3 = 2 \frac{\rho - 1}{n_s (1 + \rho)^3} n_0^2 \sin^2 \phi \tan^2 \phi \sec^2 \psi e^{i\Delta} \quad (20)$$

and

$$dn_{sr} = \text{real}(dn_s) \quad \text{and} \quad dn_{si} = \text{imag}(dn_s). \quad (21)$$

Here, dn_{sr} and dn_{si} are the differentials in the substrate's real and imaginary parts of refractive index. This leads to a standard deviation of the ellipsometrically measured quantities n_{sr} and n_{si} as follows:

$$\sigma_{n_{sr}} = \sqrt{\text{real}^2(a_1) \sigma_\phi^2 + \text{real}^2(a_2) \sigma_\Delta^2 + \text{real}^2(a_3) \sigma_{psi}^2} \quad (22)$$

$$\sigma_{n_{si}} = \sqrt{\text{imag}^2(a_1) \sigma_\phi^2 + \text{imag}^2(a_2) \sigma_\Delta^2 + \text{imag}^2(a_3) \sigma_{psi}^2}, \quad (23)$$

where σ_ϕ , σ_Δ , and σ_{psi} are the standard deviations of ϕ , Δ , and ψ when the measurement errors are random. This present FORTRAN program calculates the maximum uncertainty for treating systematic errors, which are more likely for an ellipsometer, and gives the uncertainties in n_{sr} and n_{si} as:

$$\delta n_{sr} = |\text{real}(a_1) \delta\psi| + |\text{real}(a_2) \delta\Delta| + |\text{real}(a_3) \delta\phi| \quad (24)$$

$$\delta n_{si} = |\text{imag}(a_1) \delta\psi| + |\text{imag}(a_2) \delta\Delta| + |\text{imag}(a_3) \delta\phi|, \quad (25)$$

where δ represents systematic measurement uncertainties.

The film-substrate uncertainty equations are more complicated but are derived as follows. Δ and ψ from eq (1) have the following functional form:

$$\Delta = \Delta(\phi, \lambda, n_0, n_f, t, n_s) \quad (26)$$

$$\psi = \psi(\phi, \lambda, n_0, n_f, t, n_s). \quad (27)$$

By taking the total differential of eqs (26) and (27) and then assuming all variations are known except the variations in film thickness, dt , and refractive index, dn_f , the following results of the solution for dt and dn_f are obtained, neglecting the variations in n_0 and λ :

$$dt = \frac{1}{k_1} [b_1 d\psi + b_2 d\Delta + b_3 d\phi + b_4 dn_{sr} + b_5 dn_{si}] \quad (28)$$

$$dn_f = \frac{1}{k_1} [c_1 d\psi + c_2 d\Delta + c_3 d\phi + c_4 dn_{sr} + c_5 dn_{si}], \quad (29)$$

where

$$b_1 = \frac{\partial \Delta}{\partial n_f} \quad (30)$$

$$b_2 = \frac{\partial \psi}{\partial n_f} \quad (31)$$

$$b_3 = \frac{\partial \Delta}{\partial \phi} \frac{\partial \psi}{\partial n_f} - \frac{\partial \psi}{\partial \phi} \frac{\partial \Delta}{\partial n_f} \quad (32)$$

$$b_4 = \frac{\partial \Delta}{\partial n_{sr}} \frac{\partial \psi}{\partial n_f} - \frac{\partial \psi}{\partial n_{sr}} \frac{\partial \Delta}{\partial n_f} \quad (33)$$

$$b_5 = \frac{\partial \Delta}{\partial n_{si}} \frac{\partial \psi}{\partial n_f} - \frac{\partial \psi}{\partial n_{si}} \frac{\partial \Delta}{\partial n_f} \quad (34)$$

$$c_1 = \frac{\partial \Delta}{\partial t} \quad (35)$$

$$c_2 = \frac{\partial \psi}{\partial t} \quad (36)$$

$$c_3 = \frac{\partial \Delta}{\partial \phi} \frac{\partial \psi}{\partial t} - \frac{\partial \psi}{\partial \phi} \frac{\partial \Delta}{\partial t} \quad (37)$$

$$c_4 = \frac{\partial \Delta}{\partial n_{sr}} \frac{\partial \psi}{\partial t} - \frac{\partial \psi}{\partial n_{sr}} \frac{\partial \Delta}{\partial t} \quad (38)$$

$$c_5 = \frac{\partial \Delta}{\partial n_{si}} \frac{\partial \psi}{\partial t} - \frac{\partial \psi}{\partial n_{si}} \frac{\partial \Delta}{\partial t} \quad (39)$$

and

$$k_1 = \frac{\partial \psi}{\partial n_f} \frac{\partial \Delta}{\partial t} - \frac{\partial \Delta}{\partial n_f} \frac{\partial \psi}{\partial t}. \quad (40)$$

The uncertainties for the two measured quantities t and n_f are then

$$\delta t = \frac{1}{|k_1|} [|b_1 \delta \psi| + |b_2 \delta \Delta| + |b_3 \delta \phi| + |b_4 \delta n_{sr}| + |b_5 \delta n_{si}|] \quad (41)$$

$$\delta n_f = \frac{1}{|k_1|} [|c_1 \delta \psi| + |c_2 \delta \Delta| + |c_3 \delta \phi| + |c_4 \delta n_{sr}| + |c_5 \delta n_{si}|]. \quad (42)$$

The desired partial derivatives contained in eqs (30) through (40) are derived explicitly from eq (1) by first taking the partial derivative of eq (1) with respect to either t , n_f , ϕ , n_{sr} , or n_{si} . For example, to find the quantities $\frac{\partial \psi}{\partial t}$ and $\frac{\partial \Delta}{\partial t}$, one gets[6]:

$$\left[\sec^2 \psi \frac{\partial \psi}{\partial t} + i \tan \psi \frac{\partial \Delta}{\partial t} \right] e^{i\Delta} = \frac{\partial \left(\frac{R_p}{R_s} \right)}{\partial t} = \tan \psi e^{i\Delta} C, \quad (43)$$

where C is defined as

$$C = \frac{1}{R_p} \frac{\partial R_p}{\partial t} - \frac{1}{R_s} \frac{\partial R_s}{\partial t}. \quad (44)$$

By separating eq (43) into its real and imaginary parts, one obtains for the solutions for $\frac{\partial \psi}{\partial t}$ and $\frac{\partial \Delta}{\partial t}$:

$$\frac{\partial \psi}{\partial t} = \frac{\sin 2\psi}{2} \text{real}(C) \quad (45)$$

and

$$\frac{\partial \Delta}{\partial t} = \text{imag}(C). \quad (46)$$

The following calculation allows one to determine the uncertainties in Δ and ψ when performing the conventional null ellipsometric measurement in one zone with an ideal ellipsometer having a simple quarter-wave plate. The uncertainties in the calculated values for Δ and ψ can be calculated from the uncertainties in the polarizer and analyzer null positions, P and A , and the quarter-wave plate's azimuth angle, Q , transmittance ratio, T_c , and relative phase retardation, Δ_c , uncertainties. From eq (1)

$$\Delta = \tan^{-1} \left[\frac{\text{imag}(\rho)}{\text{real}(\rho)} \right] \quad (47)$$

and

$$\psi = \tan^{-1} \sqrt{\text{imag}^2(\rho) + \text{real}^2(\rho)}. \quad (48)$$

For this ellipsometer [7],

$$\rho = \frac{\tan A [\tan Q + \rho_c \tan(P - Q)]}{\rho_c \tan Q \tan(P - Q) - 1} = \rho_r + i \rho_i, \quad (49)$$

where ρ_c for the waveplate is given by

$$\rho_c = T_c e^{i\Delta_c}. \quad (50)$$

ρ_r and ρ_i are the real and imaginary parts of ρ . ρ_c is a complex number characterizing waveplate by the ratio, T_c , of the transmittance along its fast axis to the transmittance along its slow axis and the relative phase retardation, Δ_c , between these two axes.

The differentials of Δ and ψ are given by

$$d\Delta = \frac{1}{k_2} [d_1 dP + d_2 dA + d_3 dQ + d_4 dT_c + d_5 d\Delta_c] \quad (51)$$

and

$$d\psi = \frac{1}{k_3} [e_1 dP + e_2 dA + e_3 dQ + e_4 dT_c + e_5 d\Delta_c], \quad (52)$$

where

$$d_1 = \frac{\partial \rho_i}{\partial P} - \frac{\rho_i}{\rho_r} \frac{\partial \rho_r}{\partial P} \quad (53)$$

$$d_2 = \frac{\partial \rho_i}{\partial A} - \frac{\rho_i}{\rho_r} \frac{\partial \rho_r}{\partial A} \quad (54)$$

$$d_3 = \frac{\partial \rho_i}{\partial Q} - \frac{\rho_i}{\rho_r} \frac{\partial \rho_r}{\partial Q} \quad (55)$$

$$d_4 = \frac{\partial \rho_i}{\partial T_c} - \frac{\rho_i}{\rho_r} \frac{\partial \rho_r}{\partial T_c} \quad (56)$$

$$d_5 = \frac{\partial \rho_i}{\partial \Delta_c} - \frac{\rho_i}{\rho_r} \frac{\partial \rho_r}{\partial \Delta_c} \quad (57)$$

$$e_1 = \rho_i \frac{\partial \rho_i}{\partial P} + \rho_r \frac{\partial \rho_r}{\partial P} \quad (58)$$

$$e_2 = \rho_i \frac{\partial \rho_i}{\partial A} + \rho_r \frac{\partial \rho_r}{\partial A} \quad (59)$$

$$e_3 = \rho_i \frac{\partial \rho_i}{\partial Q} + \rho_r \frac{\partial \rho_r}{\partial Q} \quad (60)$$

$$e_4 = \rho_i \frac{\partial \rho_i}{\partial T_c} + \rho_r \frac{\partial \rho_r}{\partial T_c} \quad (61)$$

$$e_5 = \rho_i \frac{\partial \rho_i}{\partial \Delta_c} + \rho_r \frac{\partial \rho_r}{\partial \Delta_c} \quad (62)$$

and

$$k_2 = \rho_r + \frac{\rho_i^2}{\rho_r} \quad (63)$$

$$k_3 = (1 + \rho_r^2 + \rho_i^2) \sqrt{(\rho_r^2 + \rho_i^2)}. \quad (64)$$

This gives the uncertainties in Δ and ψ for the conventional null ellipsometer as

$$\delta \Delta = \frac{1}{|k_2|} [|d_1 \delta P| + |d_2 \delta A| + |d_3 \delta Q| + |d_4 \delta T_c| + |d_5 \delta \Delta_c|] \quad (65)$$

$$\delta \psi = \frac{1}{|k_3|} [|e_1 \delta P| + |e_2 \delta A| + |e_3 \delta Q| + |e_4 \delta T_c| + |e_5 \delta \Delta_c|]. \quad (66)$$

The above equations are explicitly contained in the FORTRAN program which is described in the next section. These calculated uncertainties can be listed or plotted as a function of the angle of incidence, usually the one most easily varied ellipsometric parameter.

Program Description

The FORTRAN program which appears in the appendix of this report is described by the line numbers at the left-hand margin. In addition, a flow chart showing the program input and output data is given in figure 1. The program contains the introduction and declarations, line numbers 1 to 60; the places to enter in input data, line numbers 61 to

249; the theoretical calculations at every one degree of incident angle, line numbers 250 to 690; the program printout and graphics, lines numbers 691 to 757; and three short trigonometric subroutines. Except for the graphics subroutines for a Digital Equipment Corp. VAX-11 computer,* a FORTRAN IV or FORTRAN 77 compiler may be used for the program. A brief listing of some of the program line numbers with further explanation are as follows. The variables that need to be abbreviated or changed for the FORTRAN program are shown in parentheses.

Line Numbers Description

69 to 75	choose between the bare- or film-substrate models
101 to 105	if bare substrate, film thickness is zero and
-	refractive index equals that of air
153 to 161	choose between entering conventional null data
-	or errors in Δ (DEL) and ψ (PSI)
248	defines substrate refractive index n_s (NS) in eq (12)
257	defines incident angle in radians, ϕ (PHI)
266	calculates eq (10) in text
283 to 286	calculates eqs (6), (7), (8), and (9)
303 to 304	calculates eqs (1), (2), (3), (4), and (5)
308 to 313	calculates Δ , ψ , and ρ (RHO) in eqs
-	(11), (26), and (27)
314	calculates ρ_c (RHOC) of the waveplate in eq (50)
333 to 340	calculate positions of the polarizer and analyzer at
-	null for zones one and three
410 to 424	$\delta\Delta$ (DDEL) and $\delta\psi$ (DPSI) are calculated for the null ellipsometer
-	case, eqs (63) and (64). In some variables
-	ρ_r (RHOR) and ρ_i (RHOI) are shortened to (RI) and (RR).
443 to 449	calculates $\frac{\partial\psi}{\partial t}$ (DPSIDT) and $\frac{\partial\Delta}{\partial t}$ (DDELDT) needed
-	in eqs (35) to (40)
506 to 513	calculates $\frac{\partial\psi}{\partial n_f}$ (DPSIDN) and $\frac{\partial\Delta}{\partial n_f}$ (DDELDN)
565 to 573	calculates $\frac{\partial\psi}{\partial\phi}$ (DPSIDO) and $\frac{\partial\Delta}{\partial\phi}$ (DDELDO)
596 to 603	calculates $\frac{\partial\psi}{\partial n_{s,r}}$ (DPSIDNR) and $\frac{\partial\Delta}{\partial n_{s,r}}$ (DDELNR)
626 to 633	calculates $\frac{\partial\psi}{\partial n_{s,i}}$ (DPSIDNI) and $\frac{\partial\Delta}{\partial n_{s,i}}$ (DDELNI)
636 to 640	calculates k_1 (K1) in eq (40)
644 to 661	calculates δt (DT) in eq (41) and δn_f (DNF) in eq (42)
665 to 691	calculates $\delta n_{s,r}$ (DNSR) and $\delta n_{s,i}$ (DNSI) in eqs (24) and (25)

* Certain commercial equipment, instruments, or materials are identified in this paper in order to adequately specify the experimental procedure. Such identification does not imply recommendation or endorsement by the National Bureau of Standards, nor does it imply that the materials or equipment identified are necessarily the best available for the purpose.

See the program listing itself for the complete description.

Example Program Outputs

The following figures show how the uncertainties in refractive index and thickness vary with the angle of incidence. Figure 2 shows the uncertainties in refractive index and thickness for a 100-nm silicon dioxide film on silicon. There is relatively little angular variation for angles of incidence from 25 deg to 80 deg, and for uncertainties in the angle of incidence and Δ and ψ of 0.01 deg, the thickness and refractive index of the 100-nm film can be measured quite accurately. Figure 3 shows the variation of thickness and refractive index uncertainty for a thin 10-nm silicon dioxide film on silicon. Here, for uncertainties in the angle of incidence of 0.001 deg and Δ and ψ of 0.05 deg, the principal angle of incidence at 75.5 deg is the preferred angle of incidence to make the measurement. Figure 4 plots the uncertainties for a 280-nm silicon dioxide film thickness near the first order film-phase period occurring at about 70 deg. Although an accurate measurement cannot be made near 70 deg, one can still make a reasonably accurate measurement at an angle of incidence around 25 deg. Figure 5 plots for a silicon nitride film on silicon the uncertainties of thickness and refractive index. This differs from a silicon dioxide film in that its higher index, 1.98, gives rise to a more accurate measurement because of its index mismatch with air, and because the 80-nm silicon nitride film has its principal angle near 15 deg which is near the condition for maximum accuracy. Figure 6 shows how both the real and imaginary parts of the refractive index uncertainty vary as a function of the angle of incidence for the bare silicon substrate.

Conclusions

Many ellipsometers can make measurements to high precision. However, the present program allows one to calculate the maximum accuracy obtainable from any ellipsometer when performing an ellipsometric measurement using either one of two specific surface models: the refractive index of a bare substrate or the thickness and refractive index of a nonabsorbing film on a substrate. By inputting the appropriate uncertainties in the known measurement parameters, the maximum accuracy as a function of the angle of incidence can be displayed. By changing the magnitude of the input uncertainties, one can ascertain which parameter uncertainties are contributing the most to overall measurement uncertainty. When measuring an unknown bare substrate or a film of unknown thickness, one or two iterations of the input parameters, such as the incident angle, are necessary to maximize the accuracy.

An ellipsometer is an instrument that can be used to measure either the absolute optical properties of a surface or relative changes in them. Although the concern here is only with the accuracy of an absolute ellipsometric determination of these properties, because of the nonlinear nature of the electromagnetic theory that describes the measurement process, even relative changes in a surface's optical properties can be subject to large measurement error. An example of this type of measurement would be the calculated change in film thickness as a function of some growth parameter in terms of changes in Δ and ψ .

Requests for this program on recorded medium should be addressed to the author.

Acknowledgments

The author wishes to thank George A. Candela for the many enlightening discussions on ellipsometric instrumentation and theory.

References

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2. R.M.A. Azzam and N.M. Bashara, Ellipsometry and Polarized Light (North-Holland, New York, 1977), pp. 388-389.
3. D. Chandler-Horowitz, Ellipsometric Accuracy and the Principal Angle of Incidence, SPIE Vol. 342, Integrated Circuit Metrology (1982), pp. 122-123.
4. D. Chandler-Horowitz and G.A. Candela, On the Accuracy of Ellipsometric Thickness Determinations For Very Thin Films, Journal De Physique Colloque C10, Ellipsometry '83 (Dec. 1983), pp. c10-24.
5. R.M.A. Azzam and N.M. Bashara, Chapter 4.
6. J. Humlicek, Evaluation of Derivatives of Reflectance and Transmittance by Stratified Structures and Solution of the Reverse Problem of Ellipsometry, Optica Acta, 1983, vol. 30, no. 1, p. 102.
7. F.L. McCrackin, p. 23.

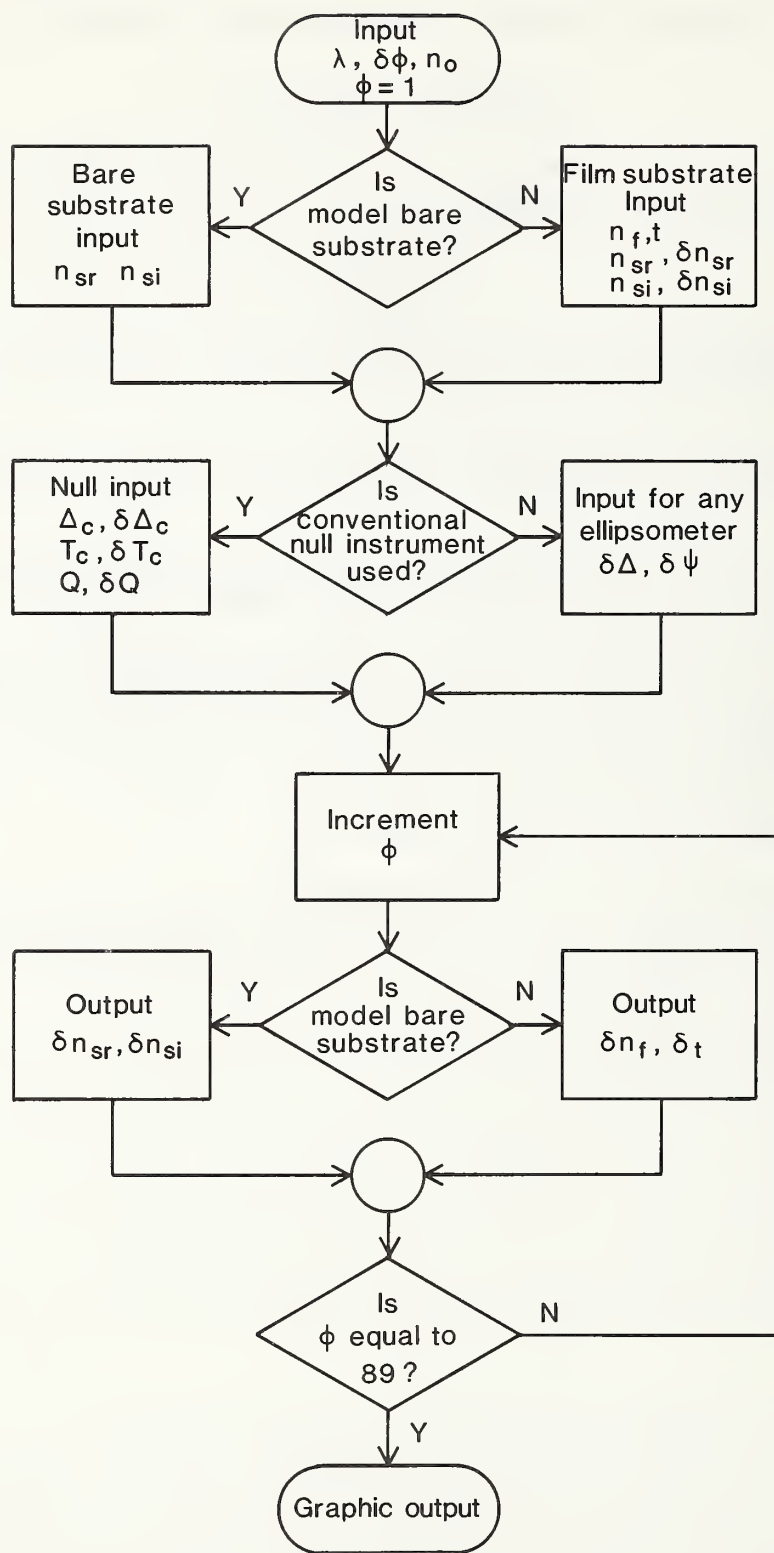


Figure 1. Program flow chart.

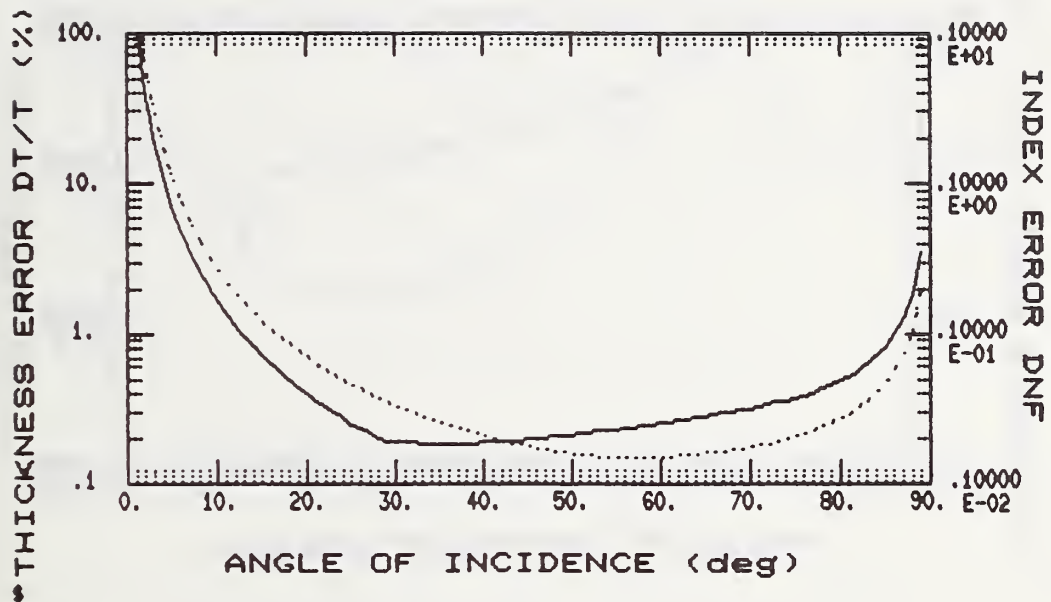


Figure 2. Plot of percent error of thickness (DT/T), solid line, and error in refractive index, dashed line, for an oxide film 100 nm thick on a silicon substrate. The input parameters are:

wavelength	632.8 nm
incident angle uncertainty	0.01 deg
film refractive index	1.46
film thickness	100 nm
substrate refractive index (real part)	3.865
uncertainty in real part	0.005
substrate refractive index (imag part)	0.018
uncertainty in imag part	0.002
uncertainty in DEL	0.05
uncertainty in PSI	0.05

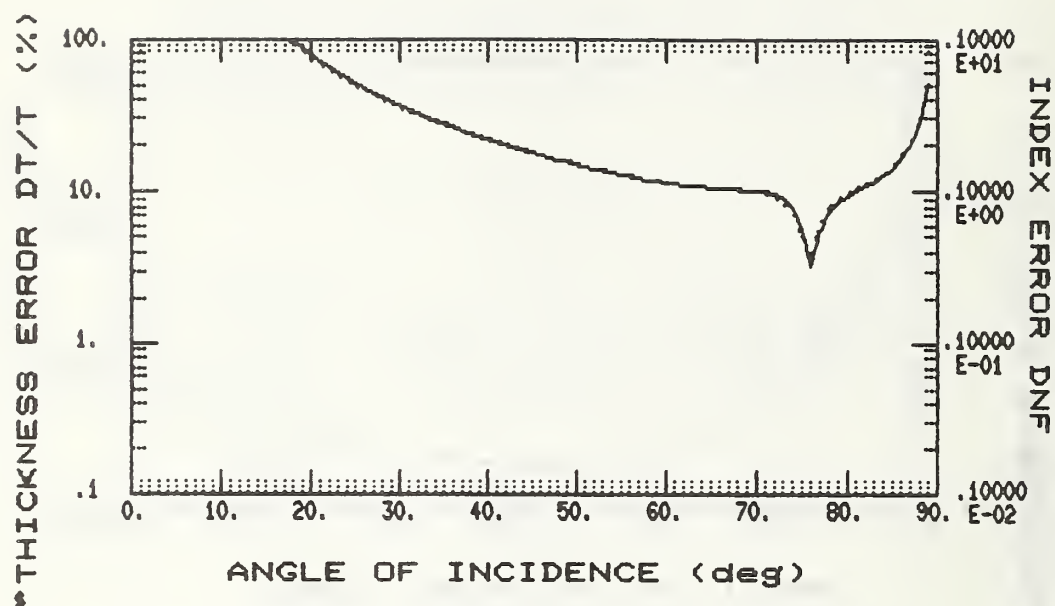


Figure 3. Plot of percent error in thickness (DT/T), solid line, and error in refractive index, dashed line, for an oxide film 10 nm thick on a silicon substrate. The input parameters are:

wavelength	632.8 nm
incident angle uncertainty	0.001 deg
film refractive index	1.46
film thickness	10 nm
substrate refractive index (real part)	3.865
uncertainty in real part	0.001
substrate refractive index (imag part)	0.018
uncertainty in imag part	0.001
uncertainty in DEL	0.02
uncertainty in PSI	0.02

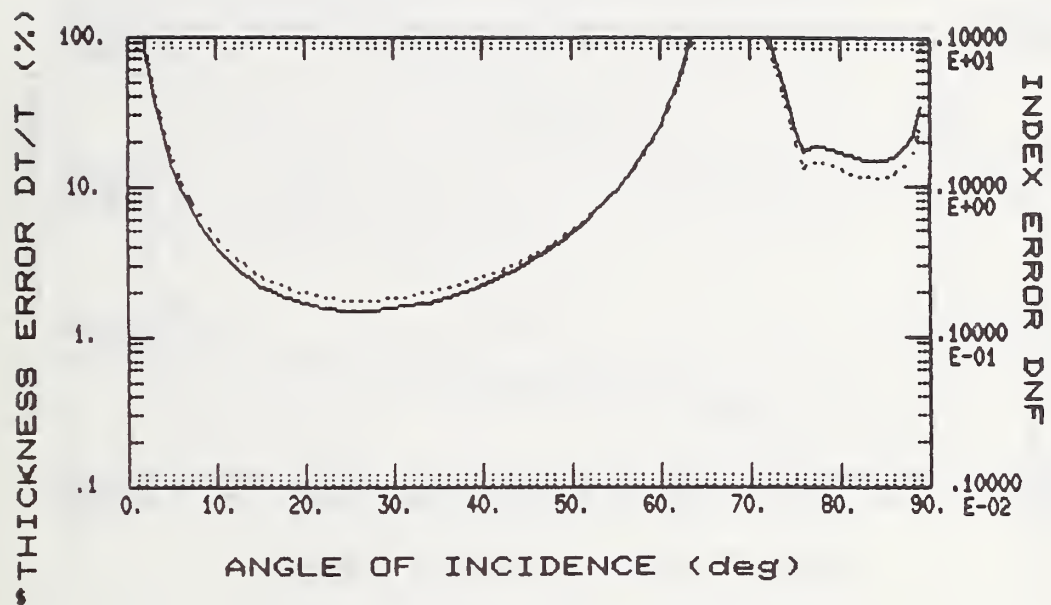


Figure 4. Plot of percent error of thickness (DT/T), solid line, and error in refractive index, dashed line, for an oxide film 280 nm thick on a silicon substrate. The input parameters are:

wavelength	632.8 nm
incident angle uncertainty	0.002 deg
film refractive index	1.46
film thickness	280 nm
substrate refractive index (real part)	3.865
uncertainty in real part	0.005
substrate refractive index (imag part)	0.018
uncertainty in imag part	0.002
uncertainty in DEL	0.02
uncertainty in PSI	0.02

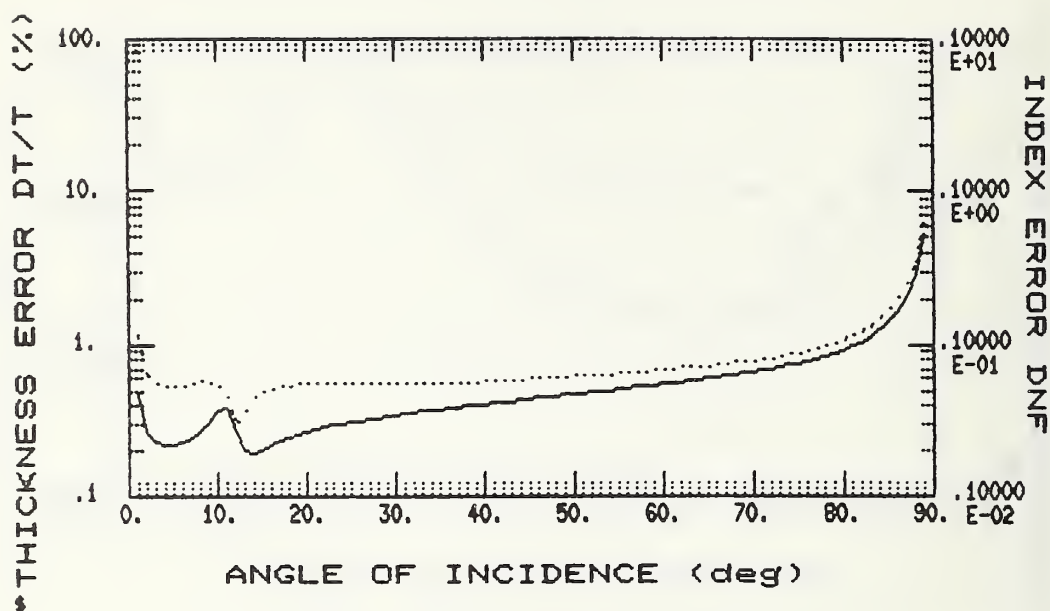


Figure 5. Plot of percent error of thickness (DT/T), solid line, and error in refractive index, dashed line, for a silicon nitride film 80 nm thick on a silicon substrate. The input parameters are:

wavelength	632.8 nm
incident angle uncertainty	0.01 deg
film refractive index	1.98
film thickness	80 nm
substrate refractive index (real part)	3.865
uncertainty in real part	0.005
substrate refractive index (imag part)	0.018
uncertainty in imag part	0.002
uncertainty in DEL	0.05
uncertainty in PSI	0.05

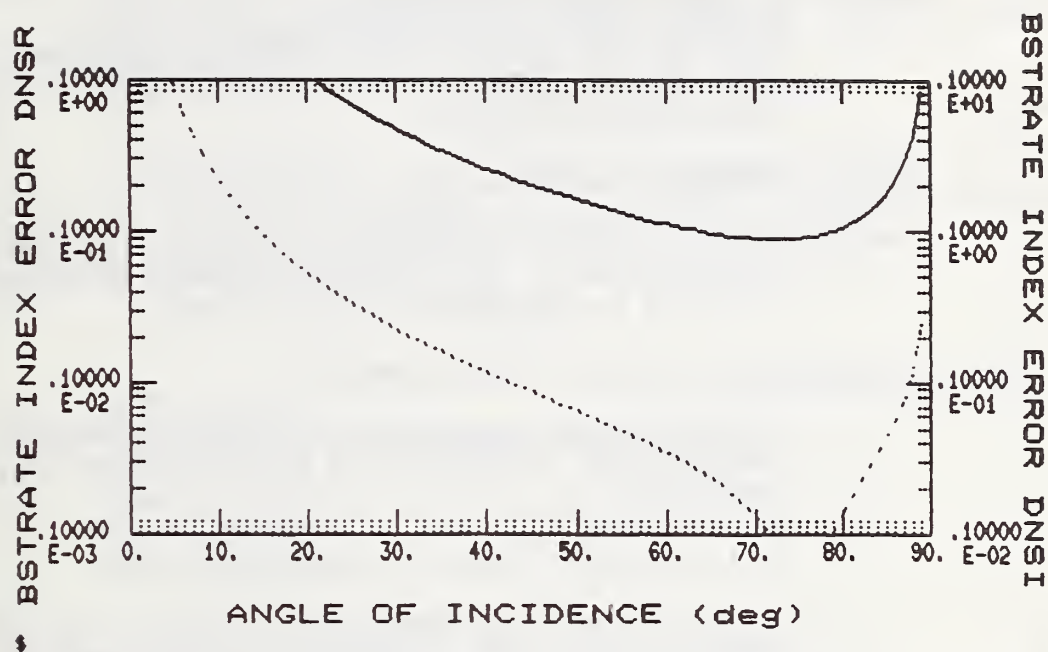


Figure 6. Plot of error in the refractive index (real part), solid line, and error in refractive index (imag part), dashed line, for a bare silicon substrate. The input parameters are:

wavelength	632.8 nm
incident angle uncertainty	0.01 deg
substrate refractive index (real part)	3.865
uncertainty in real part	0.005
substrate refractive index (imag part)	0.018
uncertainty in imag part	0.002
uncertainty in DEL	0.05
uncertainty in PSI	0.05

APPENDIX

```

0001 C      PROGRAM          ERROR.FOR
0002 C
0003 C      WRITTEN BY DEANE CHANDLER-HOROWITZ
0004 C      NATIONAL BUREAU OF STANDARDS
0005 C      SEMICONDUCTOR MATERIALS AND PROCESSING DIVISION  725
0006 C      BLDG. 225, RM. A331
0007 C      GAITHERSBURG, MD 20899
0008 C
0009 C      DATE:   NOVEMBER 19, 1984
0010 C
0011 C      PURPOSE: TO CALCULATE THE UNCERTAINTY IN THE ELLIPSOMETRIC
0012 C      DETERMINATION OF THE THICKNESS AND INDEX OF REFRACTION
0013 C      OF A FILM ON A SUBSTRATE
0014 C
0015 C                      OR
0016 C
0017 C      TO CALCULATE THE UNCERTAINTY IN THE ELLIPSOMETRIC
0018 C      DETERMINATION OF THE INDEX OF REFRACTION OF A BARE
0019 C      SUBSTRATE
0020 C
0021 C      AS A FUNCTION OF ANGLE OF INCIDENCE
0022 C
0023 C      ASSUME THE AMBIENT-FILM-SUBSTRATE MODEL OR THE BARE
0024 C      SUBSTRATE MODEL BEST DESCRIBES THE ACTUAL SURFACE
0025 C
0026 C      GIVEN THE UNCERTAINTIES IN THE ANGLE OF INCIDENCE,
0027 C      DEL AND PSI (OR IN THE CASE OF THE NULL ELLIPSOMETER,
0028 C      NULL VALUES OF POLARIZER AND ANALYSER, WAVEPLATE ANGLE,
0029 C      AND WAVEPLATE CONSTANTS), AND FOR THE BARE SUBSTRATE
0030 C      MODEL THE SUBSTRATE'S REFRACTIVE INDEX
0031 C
0032 C      ASSUME NO WAVELENGTH UNCERTAINTY
0033 C
0034 C      THIS PROGRAM VERSION CONTAINS EXPLICIT EXPRESSIONS FOR THE
0035 C      PARTIAL DERIVATIVES OF DEL AND PSI.
0036 C
0037 C -----
0038 C      MAKE NEEDED DECLARATIONS
0039 C
0040 C      REAL Q,NF,NSR,NSI,NO,X(91),YT(91),YN(91),K1
0041 C
0042 C      COMPLEX NS,CS,CRPFS,CRSFS,RP,RS,UP2,VP2,US2,VS2,EJ,AP,BP,AS,BS,
0043 C      1 DAPDT,DBPDT,DASDT,DBSDT,DRPDT,DRSDT,CT,QC,UP2DNF,VP2DNF,CPFSDN,
0044 C      2 CSFSDN,Z1,Z2,DAPDNF,DBPDNF,DASDNF,DBSDNF,DRPDNF,DRSDNF,CNF,UP2D0,
0045 C      3 VP2D0,CPFSD0,US2D0,VS2D0,CSFSD0,Y1,Y2,Y3,Y4,DAPD0,DBPD0,DASD0,
0046 C      4 DBSD0,DRPD0,DRSD0,C0,Z,RH0,RH0C,US2DNF,VS2DNF,US2DNR,VS2DNR,
0047 C      5 UP2DNR,VP2DNR,US2DNI,VS2DNI,UP2DNI,VP2DNI,CPFDNI,CPFDNR,CSFDNI,
0048 C      6 CSFDNR,DAPDNR,DAPDNI,DASDNR,DASDNI,DBSDNI,DBSDNR,DBPDNR,DBPDNI,
0049 C      7 ZA,ZB,ZC,ZD
0050 C
0051 C      LOGICAL Q1
0052 C

```

```

0053      WRITE (6,10)
0054 10     FORMAT(1X,'THIS PROGRAM, ''ERROR.FOR'', CALCULATES THE
0055      1  UNCERTAINTY IN THE FILM')
0056      WRITE (6,20)
0057 20     FORMAT(1X,'THICKNESS AND REFRACTIVE INDEX OR SUBSTRATE INDEX
0058      1  VERSUS INCIDENT ANGLE AS')
0059      WRITE (6,30)
0060 30     FORMAT(1X,'FUNCTION OF THE EXPERIMENTAL ERRORS'/)
0061      C
0062      C
0063      C      -----
0064      C      ASK THE OPERATOR FOR VALUES FOR PSI,DEL,WAVELENGTH,ANGLE OF
0065      C      INCIDENCE,NO,NF,NS, AND THEIR UNCERTAINTIES
0066      RD=57.29578
0067      C      CONVERTS DEGREES TO RADIANS
0068      C
0069      C      CHOOSE BETWEEN THE BARE OR FILM-SUBSTRATE MODEL
0070      WRITE (6,40)
0071 40     FORMAT(1X,'ENTER 1 FOR BARE SUBSTRATE')
0072      WRITE (6,50)
0073 50     FORMAT(1X,'ENTER 2 FOR FILM-SUBSTRATE')
0074      READ (5,60) II
0075 60     FORMAT(I1)
0076      C
0077      C      ENTER INPUT DATA
0078      C
0079      IF (II .EQ. 1) WRITE (4,70)
0080 70     FORMAT(T30,'SUBSTRATE REFRACTIVE INDEX UNCERTAINTY'/)
0081      IF (II .EQ. 2) WRITE (4,80)
0082 80     FORMAT(T30,'FILM INDEX AND THICKNESS UNCERTAINTY'/)
0083      C
0084      WRITE(4,90)
0085      WRITE(6,90)
0086 90     FORMAT(1X,'ENTER WAVELENGTH IN NANOMETERS')
0087      READ(5,100) WL
0088      WRITE(4,100) WL
0089 100    FORMAT(F10.2)
0090      C
0091      WRITE(4,110)
0092      WRITE(6,110)
0093 110    FORMAT(/1X,'ENTER UNCERTAINTY IN ANGLE OF INCIDENCE IN DEGREES')
0094      READ(5,120) DPHI
0095      WRITE(4,120) DPHI
0096 120    FORMAT(F10.3)
0097      DPHI=DPHI/RD
0098      C
0099      NO=1.00036
0100      C      INDEX OF AIR
0101      C      IF BARE SUBSTRATE, FILM THICKNESS IS ZERO AND
0102      C      REFRACTIVE INDEX EQUALS THAT OF AIR
0103      C
0104 125    IF (II .EQ. 1) NF=NO

```

```

0105      IF (II .EQ. 1) T=0
0106 126    IF (II .EQ. 1) GOTO 170
0107      WRITE(4,130)
0108      WRITE(6,130)
0109 130    FORMAT(/1X,'ENTER INDEX OF REFRACTION OF FILM (NON-ABSORBING)')
0110      READ(5,140) NF
0111      WRITE(4,140) NF
0112 140    FORMAT(F9.4)
0113      C
0114      WRITE(4,150)
0115      WRITE(6,150)
0116 150    FORMAT(/1X,'ENTER THICKNESS OF FILM IN NANOMETERS')
0117      READ(5,160) T
0118      WRITE(4,160) T
0119 160    FORMAT(F10.2)
0120      C
0121 170    WRITE(4,180)
0122      WRITE(6,180)
0123 180    FORMAT(/1X,'ENTER REAL PART OF SUBSTRATE REFRACT INDEX')
0124      READ(5,190) NSR
0125      WRITE(4,190) NSR
0126 190    FORMAT(F9.4)
0127      C
0128      IF (II .EQ. 1) GOTO 220
0129      WRITE(4,200)
0130      WRITE(6,200)
0131 200    FORMAT(/1X,'ENTER UNCERTAINTY IN REAL PART OF SUBSTRATE
0132 1 REFRACTIVE INDEX')
0133      READ(5,210) DNSR
0134      WRITE(4,210) DNSR
0135 210    FORMAT(F9.4)
0136      C
0137 220    WRITE(4,230)
0138      WRITE(6,230)
0139 230    FORMAT(/1X,'ENTER IMAGINARY PART OF SUBSTRATE REFRACT INDEX')
0140      READ(5,240) NSI
0141      WRITE(4,240) NSI
0142 240    FORMAT(F9.4)
0143      C
0144      IF (II .EQ. 1) GOTO 270
0145      WRITE(4,250)
0146      WRITE(6,250)
0147 250    FORMAT(/1X,'ENTER UNCERTAINTY IN IMAGINARY PART OF SUBSTRATE
0148 1 REFRACTIVE INDEX')
0149      READ(5,260) DNSI
0150      WRITE(4,260) DNSI
0151 260    FORMAT(F9.4)
0152      C
0153      C      CHOOSE BETWEEN ENTERING CONVENTIONAL NULL DATA
0154      C      OR ERRORS IN DEL AND PSI
0155      C
0156 270    WRITE(6,280)

```

```

0157 280 FORMAT(/1X,'DO YOU HAVE NULL DATA AVAILABLE? (T/F)')
0158 READ(5,290) Q1
0159 290 FORMAT(L1)
0160 C
0161 IF (Q1 .EQ. .FALSE.) GOTO 460
0162 WRITE(4,300)
0163 WRITE(6,300)
0164 300 FORMAT(/1X,'ENTER UNCERTAINTY FOR POLARIZER NULL IN DEGREES')
0165 READ(5,310) DP
0166 WRITE(4,310) DP
0167 310 FORMAT(F9.3)
0168 DP=DP/RD
0169 C
0170 WRITE(4,320)
0171 WRITE(6,320)
0172 320 FORMAT(/1X,'ENTER UNCERTAINTY FOR ANALYSER NULL IN DEGREES')
0173 READ(5,330) DA
0174 WRITE(4,330) DA
0175 330 FORMAT(F9.3)
0176 DA=DA/RD
0177 C
0178 WRITE(4,340)
0179 WRITE(6,340)
0180 340 FORMAT(/1X,'ENTER THE WAVEPLATE RETARDATION IN DEGREES')
0181 READ(5,350) DELC
0182 WRITE(4,350) DELC
0183 350 FORMAT(F9.3)
0184 DELC=DELC/RD
0185 C
0186 WRITE(4,360)
0187 WRITE(6,360)
0188 360 FORMAT(/1X,'ENTER THE WAVEPLATE RETARDATION UNCERTAINTY IN
0189 1 DEGREES')
0190 READ(5,370) DDELC
0191 WRITE(4,370) DDELC
0192 370 FORMAT(F9.3)
0193 DDELC=DDELC/RD
0194 C
0195 WRITE(4,380)
0196 WRITE(6,380)
0197 380 FORMAT(/1X,'ENTER THE WAVEPLATE TRANSMISSION COEFF.')
```

```

0198 READ(5,390) TC
0199 WRITE(4,390) TC
0200 390 FORMAT(F10.5)
0201 C
0202 WRITE(4,400)
0203 WRITE(6,400)
0204 400 FORMAT(/1X,'ENTER THE WAVEPLATE TRANS. COEFF. UNCERTAINTY')
0205 READ(5,410) DTC
0206 WRITE(4,410) DTC
0207 410 FORMAT(F10.5)
0208 C

```

```

0209      WRITE(4,420)
0210      WRITE(6,420)
0211 420    FORMAT(/1X,'ENTER THE WAVEPLATE AZIMUTH ANGLE (ie +-45 deg)')
0212      READ(5,430) Q
0213      WRITE(4,430) Q
0214 430    FORMAT(F9.3)
0215      Q=Q/RD
0216      C
0217      WRITE(4,440)
0218      WRITE(6,440)
0219 440    FORMAT(/1X,'ENTER THE WAVEPLATE AZIMUTH ANGLE UNCERTAINTY
0220      1 IN DEGREES')
0221      READ(5,450) DQ
0222      WRITE(4,450) DQ
0223 450    FORMAT(F9.3)
0224      DQ=DQ/RD
0225      C
0226      C
0227      GOTO 1000
0228      C
0229      C          ERRORS IN DEL AND PSI GIVEN
0230 460    WRITE(4,470)
0231      WRITE(6,470)
0232 470    FORMAT(/1X,'ENTER UNCERTAINTY IN DEL IN DEGREES')
0233      READ(5,480) DDEL
0234      WRITE(4,480) DDEL
0235 480    FORMAT(F10.3)
0236      DDEL=DDEL/RD
0237      C
0238      WRITE(4,490)
0239      WRITE(6,490)
0240 490    FORMAT(/1X,'ENTER UNCERTAINTY IN PSI IN DEGREES')
0241      READ(5,500) DPSI
0242      WRITE(4,500) DPSI
0243 500    FORMAT(F10.3)
0244      DPSI=DPSI/RD
0245      C
0246      C          REFRACTIVE INDEX OF SUBSTRATE, NS AS IN EQUATION (12)
0247      C
0248 1000   NS=CMPLX(NSR,-NSI)
0249      C
0250      C          -----
0251      C          BEGIN LOOP FOR ALL ANGLES OF INCIDENCE, EVERY DEGREE
0252      C
0253      DO 5000 I=1,89
0254      C
0255      C          INCIDENT ANGLE IN RADIANS, PHI
0256      C
0257      PHI=I/RD
0258      SO=SIN(PHI)
0259      CO=COS(PHI)
0260      YY=NO*SO

```

```

0261      CF=SQRT(1.-(YY/NF)**2)
0262      CS=CSQRT(1.-(YY/NS)**2)
0263      C
0264      C      DEFINE BETA,B AS IN EQUATION (10)
0265      C
0266      B=8.*ATAN(1.)*T/WL*NF*CF
0267      C
0268      C      CALC FRESNEL EQUATIONS
0269      C      BREAK UP INTO SMALLER PIECES
0270      C
0271      UP1=NF*CO-N0*CF
0272      VP1=NF*CO+N0*CF
0273      UP2=NS*CF-NF*CS
0274      VP2=NS*CF+NF*CS
0275      US1=N0*CO-NF*CF
0276      VS1=N0*CO+NF*CF
0277      US2=NF*CF-NS*CS
0278      VS2=NF*CF+NS*CS
0279      C
0280      C      CALC THE FRESNEL COEFFICIENTS RPOF AND RSOF, EQS.
0281      C      (6) AND (7) AND CRPFS AND CRSFS IN EQS. (8) AND (9)
0282      C
0283      RPOF=UP1/VP1
0284      CRPFS=UP2/VP2
0285      RSOF=US1/VS1
0286      CRSFS=US2/VS2
0287      C
0288      C      DEFINE EJ, IMAGINARY EXPONENT E TO THE -2*B
0289      C
0290      Z=CMPLX(0.,-2.*B)
0291      EJ=CEXP(Z)
0292      C
0293      C
0294      C
0295      AP=RPOF+CRPFS*EJ
0296      BP=1+RPOF*CRPFS*EJ
0297      AS=RSOF+CRSFS*EJ
0298      BS=1+RSOF*CRSFS*EJ
0299      C
0300      C      CALC RP AND RS FOR THE BARE SUBSTRATE MODEL, EQS. (2), (3)
0301      C      AND FOR THE FILM-SUBSTRATE MODEL, EQS. (4) AND (5)
0302      C
0303      RP=AP/BP
0304      RS=AS/BS
0305      C
0306      C      CALC DEL AND PSI FROM INPUT PARAMETERS
0307      C
0308      PSI=ATAN(CABS(RP/RS))
0309      DEL=ATAN2(AIMAG(RP/RS),REAL(RP/RS))
0310      C
0311      C      DEFINITION OF RHO, RP/RS AS IN EQUATION (1)
0312      C

```

```

0313      RHO=RP/RS
0314      RHOC=TC*CEXP((0.,-1.)*DELC)
0315      C
0316      C -----
0317      C   IF ERRORS IN DEL AND PSI GIVEN JUMP AHEAD
0318      C   IF (Q1 .EQ. .FALSE.) GOTO 1150
0319      C
0320      C   FOR CONVENTIONAL NULL ELLISOMETER CALCULATE NULL CONDITIONS
0321      C   FOR ZONE 1 -- BEGIN CALC FOR DDEL AND DPSI
0322      C
0323      C   IF (ABS(DELC) .LT. 1.0E-8) GOTO 1100
0324      C   R=(TAN(Q)*SIN(DELC-DELC)-SIN(DELC+DELC)/TAN(Q))/2./SIN(DELC)
0325      C
0326      C   TP1=(-R+SQRT(R*R+1))/TC
0327      C   TP2=(-R-SQRT(R*R+1))/TC
0328      C   P1=ATAN(TP1)+Q
0329      C   P3=ATAN(TP2)+Q
0330      C   A1=ATAN(REAL(RHO*(TP1*TAN(Q)*RHOC-1.)/(TAN(Q)+TP1*RHOC)))
0331      C   A3=ATAN(REAL(RHO*(TP2*TAN(Q)*RHOC-1.)/(TAN(Q)+TP2*RHOC)))
0332      C   GOTO 1110
0333      1100      C   P1=Q
0334      C   P3=Q-90./RD
0335      C   A1=ATAN(REAL(RHO/TAN(Q)))
0336      C   A3=ATAN(REAL(RHO*TAN(Q)))
0337      1110      C   P1=AMOD(P1+360./RD,180./RD)
0338      C   A1=AMOD(A1+360./RD,180./RD)
0339      C   P3=AMOD(P3+360./RD,180./RD)
0340      C   A3=AMOD(A3+360./RD,180./RD)
0341      C
0342      C   AND NOW FOR THE ERRORS IN DEL AND PSI
0343      C   ZONE 1
0344      C   P=P1
0345      C   A=A1
0346      C
0347      C   DEFINE QUARTER-WAVE PLATE AZIMUTH ANGULAR QUANTITIES
0348      C
0349      C   TQ=TAN(Q)
0350      C   TQ2=TAN(Q)*TAN(Q)
0351      C   TPQ=TAN(P-Q)
0352      C   TPQ2=TAN(P-Q)*TAN(P-Q)
0353      C   SQ=SEC(Q)
0354      C   SQ2=SEC(Q)*SEC(Q)
0355      C   SPQ=SEC(P-Q)
0356      C   SPQ2=SEC(P-Q)*SEC(P-Q)
0357      C
0358      C   CALC RHOR AND RHOI AS IN EQN. (31)
0359      C
0360      C   DD=TC*TC*TQ2*TPQ2+1+2.*TC*TQ*TPQ*COS(DELC)
0361      C   RHOR=(TAN(A)/DD)*(-TQ+TC*TC*TQ*TPQ2+TQ2*TC*TPQ*COS(DELC)
0362      1 -TC*TPQ*COS(DELC))
0363      C   RHOI=(TAN(A)/DD)*(-TQ2*TC*TPQ*SIN(DELC)-TC*TPQ*SIN(DELC))
0364      C

```

```

0365 C      CALC ALL PARTIAL DERIVATIVES NEEDED IN EQNS. (33) AND (34)
0366 C
0367 C      DRRDA=dRHOR/dA, DRIDA=dRHOI/dA
0368 C
0369 C      DRRDA=2.*RHOR/SIN(2.*A)
0370 C      DRIDA=2.*RHOI/SIN(2.*A)
0371 C
0372 C      DRRDP=dRHOR/dP, DRIDP=dRHOI/dP
0373 C
0374 C      DRRDP=TAN(A)*SPQ2*TC*(TC*TQ*2.*TPQ+COS(DELC)*(TQ2-1.))/DD
0375 C      DRRDP=DRRDP-RHOR*2.*SPQ2*TQ*TC*(TC*TQ*TPQ+COS(DELC))/DD
0376 C      DRIDP=TAN(A)*SIN(DELC)*TC*SPQ2*(-TQ-1.)/DD
0377 C      DRIDP=DRIDP-RHOI*2.*SPQ2*TQ*TC*(TC*TQ*TPQ+COS(DELC))/DD
0378 C
0379 C      DRRDQ=dRHOR/dQ, DRIDQ=dRHOI/dQ
0380 C
0381 C      DRRDQ=TAN(A)*(-SQ2*TC*TC*(SQ2*TPQ2-TQ*2.*TPQ*SPQ2)+TC
0382 1 *COS(DELC)*(2.*TQ*SQ2*TPQ-TQ2*SPQ2)+TC*SPQ2*COS(DELC))/DD
0383 C      DRRDQ=DRRDQ-RHOR*(TC*TC*(2.*TQ*SQ2*TPQ2-2.*TQ2*TPQ*SPQ2)+
0384 1 2.*TC*COS(DELC)*(SQ2*TPQ-TQ*SPQ2))/DD
0385 C
0386 C      DRIDQ=TAN(A)*SIN(DELC)*TC*(-2.*TQ*SQ2*TPQ+TQ2*SPQ2+SPQ2)/DD
0387 C      DRIDQ=DRIDQ-RHOI*(TC*TC*(2.*TQ*SQ2*TPQ2-2.*TQ2*TPQ*SPQ2)+2.*TC*
0388 1 COS(DELC)*(SQ2*TPQ-TQ*SPQ2))/DD
0389 C
0390 C      DRRDTC=dRHOR/dTC, DRIDTC=dRHOI/dTC
0391 C
0392 C      DRRDTC=TAN(A)*(2.*TC*TQ*TPQ2+TQ2*TPQ*COS(DELC)-TPQ*COS(DELC))
0393 1 /DD-RR*(2.*TC*TQ2*TPQ2+2.*TQ*TPQ*COS(DELC))/DD
0394 C
0395 C      DRIDTC=TAN(A)*(-TQ2*TPQ*SIN(DELC)-TPQ*SIN(DELC))/DD-RHOI*(2.*
0396 1 TC*TQ2*TPQ2+2.*TQ*TPQ*COS(DELC))/DD
0397 C
0398 C      DRRDDC=dRHOR/dDELC, DRIDDC=dRHOI/dDELC
0399 C
0400 C      DRRDDC=-TAN(A)*SIN(DELC)*(TQ2*TC*TPQ-TC*TPQ)/DD+RHOR*SIN(DELC)
0401 1 *2.*TC*TQ*TPQ/DD
0402 C
0403 C      DRIDDC=-TAN(A)*COS(DELC)*(TQ2*TC*TPQ+TC*TPQ)/DD+RHOI*SIN(DELC)
0404 1 *2.*TC*TQ*TPQ/DD
0405 C
0406 C      DDEL=dDEL, DPSI=dPSI AS IN EQNS. (33) AND (34) DUE TO ERRORS
0407 C      IN THE QUARTER-WAVE PLATE AND POLARIZER AND ANALYSER NULL
0408 C      POSITIONS FOR THE CONVENTIONAL NULL ELLIPSOMETRIC METHOD.
0409 C
0410 C      DDEL=(DRIDP-RHOI*DRRDP/RHOR)**2*DP*DP
0411 C      DDEL=DDEL+(DRIDA-RHOI*DRRDA/RHOR)**2*DA*DA
0412 C      DDEL=SQRT(DDEL)
0413 C      DDEL=DDEL+ABS(DRIDQ-RHOI*DRRDQ/RHOR)*DQ
0414 C      DDEL=DDEL+ABS(DRIDTC-RHOI*DRRDTC/RHOR)*DTC
0415 C      DDEL=DDEL+ABS(DRIDDC-RHOI*DRRDDC/RHOR)*DDELC
0416 C      DDEL=1/ABS(RHOR)/(1+RHOI*RHOI/RHOR/RHOR)*DDEL

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0417 C
0418 DPSI=(RHOI*DRIDP+RHOR*DRRDP)**2*DP*DP
0419 DPSI=DPSI+(RHOI*DRIDA+RHOR*DRRDA)**2*DA*DA
0420 DPSI=SQRT(DPSI)
0421 DPSI=DPSI+ABS(RHOI*DRIDQ+RHOR*DRRDQ)*DQ
0422 DPSI=DPSI+ABS(RHOI*DRIDTC+RHOR*DRRDC)*DTC
0423 DPSI=DPSI+ABS(RHOI*DRIDDC+RHOR*DRRDC)*DDEL
0424 DPSI=1/(1+RHOR*RHOR+RHOI*RHOI)/SQRT(RHOR*RHOR+RHOI*RHOI)*DPSI
0425 C
0426 C -----
0427 1150 CONTINUE
0428 C COME HERE FOR DEL,PSI ERROR INPUT
0429 IF (II .EQ. 1) GOTO 1300
0430 C
0431 C BEGIN UNCERTAINTY CALC HERE FOR FILM-SUBSTRATE MODEL
0432 C
0433 C CALC PARTIAL DIFFERENTIALS OF B,AP,BP,AS,BS WITH RESPECT TO T
0434 C DBDT=dB/dT,DAPDT=dAP/dT,DBPDT=dBP/dT,DASDT=dAS/dT,DBSDT=dBS/dT
0435 C
0436 DBDT=8.*ATAN(1.)/WL*NF*CF
0437 DAPDT=-2.*(0.,1.)*CRPFS*EJ*DBDT
0438 DBPDT=-2.*(0.,1.)*RPOF*CRPFS*EJ*DBDT
0439 DASDT=-2.*(0.,1.)*CRSFS*EJ*DBDT
0440 DBSDT=-2.*(0.,1.)*RSOF*CRSFS*EJ*DBDT
0441 C
0442 C
0443 C CALC PARTIAL DIFFERENTIALS OF PSI AND DEL WITH RESPECT TO T
0444 C DPSIDT=dPSI/dT,DDELDT=dDEL/dT AS IN EQNS (22) AND (23)
0445 C
0446 DPSIDT=SIN(2.*PSI)/2.*REAL(DAPDT/AP+DBSDT/BS-
0447 1 DASDT/AS-DBPDT/BP)
0448 C
0449 DDELDT=AIMAG(DAPDT/AP+DBSDT/BS-DASDT/AS-DBPDT/BP)
0450 C
0451 C CALC PARTIAL DIFFERENTIALS OF RP, RS AND B WITH RESPECT TO NF
0452 C
0453 C FIRST DEFINE P AND QC TO HELP WITH CALCULATIONS
0454 C
0455 P=SQRT(NF*NF-NO*NO*SO*SO)
0456 QC=CSQRT(NS*NS-NO*NO*SO*SO)
0457 C
0458 C CALC PARTIAL OF B WITH RESPECT TO NF
0459 C DBDNF=dB/dNF
0460 C
0461 DBDNF=B/NF/CF/CF
0462 C
0463 C CALC PARTIAL DIFFERENTIALS OF RPOF, CRPFS, RSOF, CRSFS
0464 C UP1DNF=dUP1/dNF,VP1DNF=dVP1/dNF,DUP2DNF=dUP2/dNF,DVP2DNF=dVP2/dNF
0465 C
0466 UP1DNF=CO-NO**3*SO*SO/NF**2/P
0467 VP1DNF=CO+NO**3*SO*SO/NF**2/P
0468 UP2DNF=NS*NO*NO*SO*SO/NF**2/P-CS

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0469      VP2DNF=NS*NO*NO*SO*SO/NF**2/P+CS
0470      C
0471      C      PARTIAL DIFFERENTIAL OF RPO1 AND CRPFS WITH RESPECT TO NF
0472      C      RPOFDN=dRPOF/dNF,CPFSDN=dCRPFS/dNF
0473      C
0474      RPOFDN=UP1DNF/VP1-VP1DNF*UP1/VP1/VP1
0475      CPFSDN=UP2DNF/VP2-VP2DNF*UP2/VP2/VP2
0476      C
0477      C      US1DNF=dUS1/dNF,VS1DNF=dVS1/dNF,US2DNF=dUS2/dNF,DVS2DNF=dVS2/dNF
0478      C
0479      US1DNF=-NF/P
0480      VS1DNF=NF/P
0481      US2DNF=NF/P
0482      VS2DNF=NF/P
0483      C
0484      C      ALL THE ABOVE PARTIALS ARE ALMOST THE SAME
0485      C
0486      C      PARTIALS OF RSOF AND CRSFS
0487      C      RSOFDN=dRSOF/dNF,CSFSDN=dCRSFS/dNF
0488      C
0489      RSOFDN=US1DNF/VS1*(1.+US1/VS1)
0490      CSFSDN=US2DNF/VS2*(1.-US2/VS2)
0491      C
0492      C      NOW GET THE PARTIALS OF AP,BP,AS,BS
0493      C      DAPDNF=dAP/dNF,DBPDNF=dBP/dNF
0494      C
0495      Z1=2.*(0.,1.)*CRPFS*EJ*DBDNF
0496      DAPDNF=RPOFDN+EJ*CPFSDN-Z1
0497      DBPDNF=EJ*(RPOF*CPFSDN+CRPFS*RPOFDN-RPOF*Z1/EJ)
0498      C
0499      C      DASDNF=dAS/dNF,DBSDNF=dBS/dNF
0500      C
0501      Z2=2.*(0.,1.)*CRSFS*EJ*DBDNF
0502      DASDNF=RSOFDN+EJ*CSFSDN-Z2
0503      DBSDNF=EJ*(RSOF*CSFSDN+CRSFS*RSOFDN-RSOF*Z2/EJ)
0504      C
0505      C
0506      C      PARTIAL DIFFERENTIALS OF PSI AND DEL WITH RESPECT TO NF
0507      C      AS IN EQNS. (21) AND (23)
0508      C      DPSIDN=dPSI/dNF,DDELDN=dDEL/dNF
0509      C
0510      DPSIDN=SIN(2.*PSI)/2.*REAL(DAPDNF/AP+DBSDNF/BS-
0511      1 DASDNF/AS-DBPDNF/BP)
0512      DDELDN=AIMAG(DAPDNF/AP+DBSDNF/BS-DASDNF/AS-
0513      1 DBPDNF/BP)
0514      C
0515      C
0516      C      DEFINE ALL PARTIAL DIFFERENTIALS WITH RESPECT TO PHI
0517      C
0518      C      PARTIAL DIFFERENTIAL OF B WITH RESPECT TO PHI
0519      C      DBD0=dB/dPHI
0520      C

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0521      DBD0=-4.*NO*NO*T*ATAN(1.)/WL*SIN(2.*PHI)/P
0522      C
0523      C      PARTIALS OF RPOF,CRPFS WITH RESPECT TO PHI
0524      C      UP1D0=dUP1/dPHI,VP1D0=dVP1/dPHI,UP2D0=dUP2/dPHI,VP2D0=dVP2/dPHI
0525      C
0526      UP1D0=-NF*SO+NO**3*SIN(2.*PHI)/2./NF/P
0527      VP1D0=-NF*SO-NO**3*SIN(2.*PHI)/2./NF/P
0528      UP2D0=-NS*NO*NO*SIN(2.*PHI)/2./NF/P+NF*NO*NO*SIN(2.*PHI)/
0529      1 2./NS/QC
0530      VP2D0=-NS*NO*NO*SIN(2.*PHI)/2./NF/P-NF*NO*NO*SIN(2.*PHI)/
0531      1 2./NS/QC
0532      C
0533      C      RPOFD0=dRPOF/dPHI,CPFSD0=dCPFS/dPHI
0534      C
0535      RPOFD0=UP1D0/VP1-VP1D0*UP1/VP1/VP1
0536      CPFSD0=UP2D0/VP2-VP2D0*UP2/VP2/VP2
0537      C
0538      C      PARTIALS OF RSOF AND CRSFS
0539      C      US1D0=dUS1/dPHI,VS1D0=dVS1/dPHI,US2D0=dUS2/dPHI,VS2D0=dVS2/dPHI
0540      C
0541      US1D0=-NO*SO+NO*NO*SIN(2.*PHI)/2./P
0542      VS1D0=-NO*SO-NO*NO*SIN(2.*PHI)/2./P
0543      US2D0=NO*NO*SIN(2.*PHI)/2.*(-1./P+1./QC)
0544      VS2D0=NO*NO*SIN(2.*PHI)/2.*(-1./P-1./QC)
0545      C
0546      C      RSOFD0=dRSOF/dPHI,CSFSD0=dCSFS/dPHI
0547      C
0548      RSOFD0=US1D0/VS1-VS1D0*US1/VS1/VS1
0549      CSFSD0=US2D0/VS2-VS2D0*US2/VS2/VS2
0550      C
0551      C      PARTIALS OF AP,BP,AS, AND BS WITH RESPECT OF PHI
0552      C      DAPD0=dAP/dPHI,DBPD0=dBP/dPHI,DASD0=dAS/dPHI,DBSD0=dBS/dPHI
0553      C
0554      Y1=2.*(0.,1.)*CRPFS*EJ*DBD0
0555      DAPD0=RPOFD0+EJ*CPFSD0-Y1
0556      Y2=2.*(0.,1.)*CRPFS*RPOF*DBD0
0557      DBPD0=EJ*(CRPFS*RPOFD0+RPOF*CPFSD0-Y2)
0558      Y3=2.*(0.,1.)*CRSFS*EJ*DBD0
0559      DASD0=RSOFD0+EJ*CSFSD0-Y3
0560      Y4=2.*(0.,1.)*CRSFS*RSOF*DBD0
0561      DBSD0=EJ*(CRSFS*RSOFD0+RSOF*CSFSD0-Y4)
0562      C
0563      C      (PARTIALS OF RP AND RS WITH RESPECT TO PHI)
0564      C
0565      C      CALC PARTIAL DIFFERENTIALS OF PSI AND DELTA WITH RESPECT TO PHI
0566      C      TRIG FUNCTIONS OF DEL AND PSI
0567      C      AS IN EQNS. (21) AND (22)
0568      C      DPSID0=dPSI/dPHI,DDELD0=dDEL/dPHI
0569      C
0570      DPSID0=SIN(2.*PSI)/2.*REAL(DAPD0/AP+DBSD0/BS-
0571      1 DASD0/AS-DBPD0/BP)
0572      DDELD0=AIMAG(DAPD0/AP+DBSD0/BS-

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0573      1 DASD0/AS-DBPD0/BP)
0574      C
0575      C      TAKE DERIVATIVES WITH RESPECT TO THE REAL PART OF THE
0576      C      SUBSTRATE REFRACTIVE INDEX, NSR
0577      C      UP2DNR=dUP2/dNSR, VP2DNR=dVP2/dNSR, US2DNR=dUS2/dNSR, VS2DNR=dVS2/dNSR
0578      C
0579      C      UP2DNR=CF+NF*YY*YY/(NS**3)/CS
0580      C      VP2DNR=CF-NF*YY*YY/(NS**3)/CS
0581      C      US2DNR=-CS+YY*YY/(NS*NS*CS)
0582      C      VS2DNR=CS-YY*YY/(NS*NS*CS)
0583      C
0584      C      CPFDNR=dCRPFS/dNSR, CSFDNR=dCRSFS/dNSR
0585      C
0586      C      CPFDNR=UP2DNR/VP2-VP2DNR*UP2/VP2/VP2
0587      C      CSFDNR=US2DNR/VS2*(1.+US2/VS2)
0588      C
0589      C      DAPDNR=dAP/dNSR, DBPDNR=dBP/dNSR, DASDNR=dAS/dNSR, DBSDNR=dBS/dNSR
0590      C
0591      C      DAPDNR=EJ*CPFDNR
0592      C      DBPDNR=EJ*RPOF*CPFDNR
0593      C      DASDNR=EJ*CSFDNR
0594      C      DBSDNR=EJ*RSOF*CSFDNR
0595      C
0596      C      CALCULATE PARTIAL DERIVATIVES OF PSI AND DEL WITH RESPECT TO NSR
0597      C      AS IN EQNS. (21) AND (22)
0598      C      DPSDNR=dPSI/dNSR, DDEDNR=dDEL/dNSR
0599      C
0600      C      DPSDNR=SIN(2.*PSI)/2.*REAL(DAPDNR/AP+DBSDNR/BS-
0601      1 DASDNR/AS-DBPDNR/BP)
0602      C      DDEDNR=AIMAG(DAPDNR/AP+DBSDNR/BS-DASDNR/AS-
0603      1 DBPDNR/BP)
0604      C
0605      C      TAKE DERIVATIVES WITH RESPECT TO THE IMAG PART OF THE
0606      C      SUBSTRATE REFRACTIVE INDEX, NSI
0607      C      UP2DNI=dUP2/dNSI, VP2DNI=dVP2/dNSI, US2DNI=dUS2/dNSI, VS2DNI=dVS2/dNSI
0608      C
0609      C      UP2DNI=(CF+NF*YY*YY/(NS**3)/CS)*(0.,-1.)
0610      C      VP2DNI=(CF-NF*YY*YY/(NS**3)/CS)*(0.,-1.)
0611      C      US2DNI=(-CS+YY*YY/(NS*NS*CS))*(0.,-1.)
0612      C      VS2DNI=(CS-YY*YY/(NS*NS*CS))*(0.,-1.)
0613      C
0614      C      CPFDNI=dCRPFS/dNSI, CSFDNI=dCRSFS/dNSI
0615      C
0616      C      CPFDNI=UP2DNI/VP2-VP2DNI*UP2/VP2/VP2
0617      C      CSFDNI=US2DNI/VS2*(1.+US2/VS2)
0618      C
0619      C      DAPDNI=dAP/dNSI, DBPDNI=dBP/dNSI, DASDNI=dAS/dNSI, DBSDNI=dBS/dNSI
0620      C
0621      C      DAPDNI=EJ*CPFDNI
0622      C      DBPDNI=EJ*RPOF*CPFDNI
0623      C      DASDNI=EJ*CSFDNI
0624      C      DBSDNI=EJ*RSOF*CSFDNI

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0625 C
0626 C PARTIAL DERIVATIVES OF PSI AND DEL WITH RESPECT TO NSI
0627 C AS IN EQNS. (21) AND (22)
0628 C  $DPSDNI = dPSI/dNSI$ ,  $DDEDNI = dDEL/dNSI$ 
0629 C
0630 C  $DPSDNI = SIN(2.*PSI)/2.*REAL(DAPDNI/AP+DBSDNI/BS-$ 
0631 1  $DASDNI/AS-DBPDNI/BP)$ 
0632 C  $DDEDNI = AIMAG(DAPDNI/AP+DBSDNI/BS-DASDNI/AS-$ 
0633 1  $DBPDNI/BP)$ 
0634 C
0635 C
0636 C FINALLY DEFINE PARTIAL OF NF, THICKNESS DENOMINATOR TERM
0637 C AS IN EQN. (23)
0638 C
0639 C
0640 C  $K1 = ABS(DPSIDN*DDELDLT - DDELDN*DPSIDT)$ 
0641 C
0642 C IF  $(K1 .EQ. 0)$   $K1 = 1.0E-35$ 
0643 C
0644 C FINAL RESULT OF SUMS IN EQNS. (21) AND (22)
0645 C
0646 C  $DET1 = ABS(DDEL*DPSIDN) + ABS(DPSI*DDELDN)$ 
0647 C  $DET2 = ABS(DDEL*DPSIDT) + ABS(DPSI*DDELDT)$ 
0648 C  $DET1 = DET1 + ABS(DPHI)*ABS(DDELDO*DPSIDN - DPSIDO*DDELDN)$ 
0649 C  $DET2 = DET2 + ABS(DPHI)*ABS(DDELDO*DPSIDT - DPSIDO*DDELDT)$ 
0650 C  $DET1 = DET1 + ABS(DNSR)*ABS(DDEDNR*DPSIDN - DPSIDNR*DDELDN)$ 
0651 C  $DET2 = DET2 + ABS(DNSR)*ABS(DDEDNR*DPSIDT - DPSIDNR*DDELDT)$ 
0652 C  $DET1 = DET1 + ABS(DNSI)*ABS(DDEDNI*DPSIDN - DPSIDNI*DDELDN)$ 
0653 C  $DET2 = DET2 + ABS(DNSI)*ABS(DDEDNI*DPSIDT - DPSIDNI*DDELDT)$ 
0654 C  $DET1 = DET1/K1$ 
0655 C  $DET2 = DET2/K1$ 
0656 C
0657 C DEFINE UNCERTAINTY DATA ARRAY
0658 C X(I) ANGLE OF INCIDENCE
0659 C  $X(I) = PHI*RD$ 
0660 C  $YT(I) = DET1*100./T$ 
0661 C  $YN(I) = DET2$ 
0662 C YT(I) % THICKNESS UNCERTAINTY YN(I) FILM INDEX UNCERTAINTY
0663 C GOTO 5000
0664 C
0665 C -----
0666 C BEGIN CALC OF UNCERTAINTIES FOR BARE SUBSTRATE MODEL
0667 C CALCULATE DNSR AND DNSI AS DERIVED IN EQUATIONS
0668 C (13) THROUGH (18)
0669 C
0670 1300 C  $ZA = (NS*NS*(1.+SEC(PHI)*SEC(PHI)) + NO*NO*(1.-SEC(PHI)*SEC(PHI)))$ 
0671 1  $/NS/TAN(PHI)$ 
0672 C
0673 C  $ZD = 2.*(RH0-1.)*NO*NO*SIN(PHI)*SIN(PHI)*TAN(PHI)*TAN(PHI)/$ 
0674 1  $NS/(1.+RH0)/(1.+RH0)/(1.+RH0)$ 
0675 C
0676 C  $ZB = ZD*RH0*(0,1.)$ 

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0677 C
0678 ZC=ZD*SEC(PSI)*SEC(PSI)*CEXP((0,1.)*DEL)
0679 C
0680 DNSR=ABS(REAL(ZA)*DPHI)+ABS(REAL(ZB)*DDEL)
0681 1 +ABS(REAL(ZC)*DPSI)
0682 C
0683 DNSI=ABS(AIMAG(ZA)*DPHI)+ABS(AIMAG(ZB)*DDEL)
0684 1 +ABS(AIMAG(ZC)*DPSI)
0685 C
0686 PUT RESULTS IN ANGLE OF INCIDENCE DATA ARRAY
0687 C
0688 X(I)=PHI*RD
0689 YT(I)=DNSR
0690 YN(I)=DNSI
0691 C
0692 C -----
0693 5000 CONTINUE
0694 C
0695 DISPLAY RESULTS NEXT
0696 C
0697 THIS PROGRAM CONTAINS A PRINTOUT OF RESULTS COMMENTED OUT
0698 AND INCLUDES VAX-11 RGL GRAPHICS TO PLOT UNCERTAINTIES AS A
0699 FUNCTION OF ANGLE OF INCIDENCE.
0700 THE GRAPHICS CAN ONLY BE USED WHEN COMPILED PROGRAM IS
0701 LINKED WITH RGL GRAPHICS SUBROUTINES
0702 C
0703 INITIALIZE GRAPHICS,CLEAR SCREEN AND TEXT,DRAW GRAPH
0704 CALL INITGR(5)
0705 CALL CLRSCR
0706 CALL CLRTXT
0707 CALL SCOLOR('GRAY3',1)
0708 CALL DPAPER('LIN',9,10,'LOG',3,9,'GRAY3')
0709 C
0710 HEADINGS FOR PRINTOUT RESULTS OF FILM-SUBSTRATE MODEL
0711 IF (II .EQ. 1) GOTO 5250
0712 C WRITE(6,5200)
0713 C WRITE(4,5200)
0714 C FORMAT(/1X,'ANGLE OF INCIDENCE (deg)',3X,'PERCENT THICKNESS UNCE
0715 1TAINTY',3X,'INDEX UNCERTAINTY'/)
0716 C
0717 LABEL GRAPHS FOR FILM-SUBSTRATE MODEL
0718 CALL LNAXIS('XB','ANGLE OF INCIDENCE (deg)',0,
0719 190.,.TRUE.)
0720 CALL SCOLOR('GRAY1',2)
0721 CALL LNAXIS('YL','THICKNESS ERROR DT/T (%)',.1,100.,
0722 1.TRUE.)
0723 CALL SCOLOR('GRAY2',3)
0724 CALL LNAXIS('YR','INDEX ERROR DNF',.001,1.,.TRUE.)
0725 GOTO 5300
0726 5250 CONTINUE
0727 C HEADING FOR PRINTOUT RESULTS OF BARE SUBSTRATE MODEL
0728 C WRITE(6,5260)

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0729 C      WRITE(4,5260)
0730 C      FORMAT(/1X,'ANGLE OF INCIDENCE (deg)',2X,'INDEX(REAL) UNCERTAIN
0731 C      1TY',2X,'INDEX(IMAGINARY) UNCERTAINTY'/)
0732 C
0733 C      LABEL GRAPHS FOR BARE SUBSTRATE MODEL
0734 C      CALL LNAXIS('XB','ANGLE OF INCIDENCE (deg)',0,
0735 C      190.,.TRUE.)
0736 C      CALL SCOLOR('GRAY1',2)
0737 C      CALL LNAXIS('YL','SUBSTRATE INDEX ERROR DNSR',.001,1.,
0738 C      1.TRUE.)
0739 C      CALL SCOLOR('GRAY2',3)
0740 C      CALL LNAXIS('YR','SUBSTRATE INDEX ERROR DNSI',.001,1.,
0741 C      1.TRUE.)
0742 C
0743 C      LIST DATA
0744 C      5300 CONTINUE
0745 C      DO 6000 J=1,89
0746 C      WRITE(4,5400) X(J),YT(J),YN(J)
0747 C      WRITE(6,5400) X(J),YT(J),YN(J)
0748 C      FORMAT(5X,F10.3,20X,F12.5,20X,F9.5)
0749 C      CONTINUE
0750 C
0751 C      GRAPH DATA
0752 C      CALL PDATA(89,X,YT,'L','GRAY1',,1,.FALSE.,,)
0753 C      CALL PDATA(89,X,YN,'R','GRAY2',,9,.FALSE.,,)
0754 C
0755 C      CALL SCOLOR('GRAY3',1)
0756 C
0757 C      END OF MAIN PROGRAM
0758 C      END

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FEDERAL INFORMATION PROCESSING STANDARD SOFTWARE SUMMARY

01. Summary date Yr. Mo. Day 8 5 0 8 0 1			02. Summary prepared by (Name and Phone) Deane Chandler-Horowitz (301) 921-3625			03. Summary action New Replacement Deletion ☒ ☐ ☐ Previous Internal Software ID		
04. Software date Yr. Mo. Day 8 5 0 6 1 0			05. Software title Semiconductor Measurement Technology: A FORTRAN Program for analysis of the uncertainty in the ellipsometric determination of the thickness and refractive index of a film on a substrate or the re-					
06. Short title ERROR.FOR fractive index of a bare substrate								
08. Software type Automated Data ☐ System ☒ Computer Program ☐ Subroutine/Module			09. Processing mode ☒ Interactive ☐ Batch ☐ Combination			10. Application area General ☐ Computer Systems Support/Utility ☒ Scientific/Engineering ☐ Bibliographic/Textual Management/ Business ☐ Process Control ☐ Other		
11. Submitting organization and address Semiconductor Electronics Division National Bureau of Standards Gaithersburg, MD 20899						12. Technical contact(s) and phone Deane Chandler-Horowitz (301) 921-3625		
13. Narrative The program performs the following functions: user can choose either the bare substrate or film substrate model; user inputs ellipsometric data (wavelength of light, angle of incidence, etc.); computes from the known input uncertainties the ellipsometric output uncertainty in either the film's thickness and refractive index or the substrate's refractive index; a graph of uncertainty as a function of angle of incidence is plotted.								
14. Keywords ellipsometry; bare-substrate model; film-substrate model; thickness uncertainty; refractive index uncertainty								
15. Computer manuf'r and model DEC VAX 11/780		16. Computer operating system VMS 4.0		17. Programing language(s) FORTRAN		18. Number of source program statements 766		
19. Computer memory requirements 55 KB		20. Tape drives one for program loading		21. Disk/Drum units none		22. Terminals 1 video VT 125		
23. Other operational requirements								
24. Software availability Available ☒ Limited ☐ In-house only ☐					25. Documentation availability Available ☒ Inadequate ☐ In-house only ☐ A user's manual is available as NBS Special Publication 400-78.			
26. FOR SUBMITTING ORGANIZATION USE								

U.S. DEPT. OF COMM. BIBLIOGRAPHIC DATA SHEET (See instructions)	1. PUBLICATION OR REPORT NO. NBS/SP-400/78	2. Performing Organ. Report No.	3. Publication Date May 1986
4. TITLE AND SUBTITLE <i>Semiconductor Measurement Technology: Analytic Analysis of Ellipsometric Errors</i>			
5. AUTHOR(S) Deane Chandler-Horowitz			
6. PERFORMING ORGANIZATION (If joint or other than NBS, see instructions) National Bureau of Standards Department of Commerce Gaithersburg, MD 20899			7. Contract/Grant No. 8. Type of Report & Period Covered Final
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10. SUPPLEMENTARY NOTES Library of Congress Catalog Card Number: 86-600541 ☐ 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) A computer program is given that contains an explicit ellipsometric error analysis. The program can identify the ellipsometric inaccuracies for any ellipsometer, can be used to determine which parameters contribute the most to the overall measurement inaccuracy, and can lead one to an optimum measurement procedure. A FORTRAN program that performs the evaluation of the partial derivative expressions needed to analyze ellipsometric measurement uncertainties is listed. The program determines the uncertainty in the calculation of the refractive index of a bare isotropic substrate or the uncertainty in the determination of the thickness and refractive index of a nonabsorbing film on a substrate of known refractive index. These are the two most commonly used surface models used in ellipsometry performed at single angle of incidence and a single wavelength. The program input parameters include the wavelength of the light, the angle of incidence and its uncertainty, and the uncertainties in the ellipsometric parameters Δ and ψ . They also include in the ambient-substrate model an estimated value for the substrate's refractive index, and in the film-substrate model the refractive index of the substrate and its uncertainty and estimated values for the film's refractive index and thickness. The case of the conventional null ellipsometer utilizing a quarter-wave plate is treated to find the uncertainties in Δ and ψ from the uncertainties in the polarizer and analyzer null values and the waveplate constants.			
12. KEY WORDS (Six to twelve entries; alphabetical order; capitalize only proper names; and separate key words by semicolons) bare substrate model; ellipsometry; film substrate model; FORTRAN program; measurement uncertainties; systematic errors.			
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