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A FORTAN IV PROGRAM FOR ELLIPSOMETER
MEASUREMENTS OF SURFACE FILMS

Robert W. Loser

Donald T. Larson

THE DOW CHEMICAL COMPANY
ROCKY FLATS DIVISION
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GOLDEN, COLORADO 80401

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A FORTRAN IV PROGRAM FOR ELLIPSOMETER MEASUREMENTS OF SURFACE FILMS

R. W. Loser and D. T. Larson

Abstract. A FORTRAN IV program is presented for use with an ellipsometer to determine the index of refraction of a surface film, the thicknesses of the surface film and the index of refraction of the substrate material. The program processes data taken by an ellipsometer which is used to measure the growth of a surface film. The ellipsometer measurements are described as input data, and refractive index and film thicknesses are described as output data. Included is a brief description of the techniques used to determine refractive index and surface film thicknesses, and a complete description of the FORTRAN IV program.

INTRODUCTION

This report describes a FORTRAN IV program which is used to analyze ellipsometer data. Ellipsometry is a useful tool to study the oxidation of metals by measuring the index of refraction and thickness of the oxide film. ^(1, 2) The determination of the refractive index and thicknesses of the oxide film, however, is a complicated and tedious procedure. The analysis of the ellipsometer measurements therefore requires a computer. A FORTRAN IV program was written to determine the index of refraction of an oxide film, the thicknesses of the oxide film, and the index of refraction of the substrate material.

The ellipsometer measures two optical parameters, psi (ψ) and delta (Δ). Psi is defined as the angle whose tangent is the amplitude ratio of the parallel and perpendicular components to the plane of incidence of the electric field vector, and delta is the phase change of these components. ⁽³⁾ Psi and delta are related to the index of refraction of the substrate, the index of refraction of a film on the substrate, and the thickness of the film. ⁽⁴⁾

Before the index of refraction and the thickness of a surface film can be determined, the index of refraction of the substrate must be calculated. The calculations are straightforward. Ellipsometric measurements of psi and delta are taken for a "clean" surface (substrate with no surface film). The values of psi and delta are then substituted into the appropriate equations to calculate the index of refraction of the substrate. ⁽⁴⁾

The calculations for the index of refraction and thicknesses of a surface film are not straightforward. There are three unknown properties of the film to determine [the real and imaginary parts of the complex index of refraction of the film ($\hat{n}_2 = n_2 - k_2 i$), and the film thickness (d_2)] from only two ellipsometric measurements (psi and delta). There are two different methods for determining these properties of the surface film.

The first method is a graphical technique. ^(3, 5) Ellipsometric measurements of psi and delta are taken for a sample with changing film thickness. A constant index of refraction is assumed. An experimental delta-versus-psi curve is drawn from these data. Then a family of theoretical delta-versus-psi curves are drawn by calculating psi and delta points with a computer using various values for the index of refraction of the surface film over a specified film thickness range. By matching the experimental curve with one of the theoretical curves, the index of refraction of the film and the thicknesses of the film can be determined. A computer program was previously written for the theoretical calculation of psi and delta, given the values for the index of refraction of the substrate and the index of refraction and thicknesses of the surface film. ⁽⁶⁾

In the second method (McCrackin and Colson) ⁽¹⁾ the best index of refraction of the surface film is selected by determining which refractive index gives the smallest

(1) E. Passaglia, R. R. Stromberg, and J. Kruger, Editors. *Ellipsometry in the Measurement of Surfaces and Thin Films*. Miscellaneous Publication 256. U.S. Department of Commerce, National Bureau of Standards, Wash. D.C., 1964.

(2) J. Kruger, *Corrosion*, 22, 88 (1966).

(3) R. J. Archer, *J. Opt. Soc. Amer.*, 52, 970 (1962).

(4) F. L. McCrackin, E. Passaglia, R. R. Stromberg, and H. L. Steinberg, *J. Res. Natl. Bur. Std.*, 67A, 363 (1963).

(5) D. T. Larson and N. W. Taylor, "Ellipsometry Studies on the Cleaning and Oxidation of Uranium," RFP-674, Rocky Flats Division, The Dow Chemical Co. June 1966.

(6) C. A. Larson, "FORTRAN II Computer Program for Analysis of Ellipsometry Data," RFP-729, Rocky Flats Division, The Dow Chemical Co., December 1966.

error in a series of experimental ellipsometric measurements (psi and delta), made on a film with changing thickness and the same refractive index. Film thicknesses are then calculated directly from the index of refraction of the substrate and the index of refraction of the surface film selected.

The general method of McCrackin and Colson⁽⁷⁾ was followed in writing the FORTRAN IV program to determine the index of refraction of the surface film and to calculate directly from the psi and delta measurements the thicknesses of the surface film. The FORTRAN IV program was written because major modifications of the McCrackin and Colson program would have been required for use on an IBM S/360-40 computer.

The FORTRAN IV program presented in this report is in four separate parts. The program:

1. Calculates the index of refraction of the substrate material.
2. Calculates the thickness of a surface film for each psi and delta measurement given the index of refraction of the substrate material and the index of refraction of the surface film.
3. Determines the index of refraction of the surface film from a given series of psi and delta measurements, then calculates film thicknesses using the index of refraction of the surface film selected and the index of refraction of the substrate material.
4. Calculates the psi and delta optical parameters given the index of refraction of the substrate material, the index of refraction of the surface film and the thicknesses of the film.

MATHEMATICAL METHODS

1. Computing the Index of Refraction of the Substrate Material

The index of refraction of the substrate material is given by $\hat{n}_3 = n_{31} - n_{32}i$, where n_{31} is the real part of the refractive index and n_{32} is the imaginary part. The calculations for n_{31} and n_{32} are based upon:

- a. The index of refraction of the surrounding medium.
- b. The angle of incidence.
- c. The psi and delta measurements made on a clean substrate surface.

The equations used to calculate n_{31} and n_{32} are given by Vasicek.⁽¹⁾

2. Computing the Thickness of a Surface Film

The thickness of a surface film can be computed using the fundamental ellipsometric equation and the exact Drude equations (McCrackin and Colson)⁽¹⁾. The calculations are based upon:

- a. The index of refraction of the surrounding medium.
- b. The angle of incidence.
- c. the wavelength of the light beam.
- d. The index of refraction of the substrate.
- e. The index of refraction of the surface film.
- f. The experimental psi and delta measurements.

The index of refraction of the substrate is given by $\hat{n}_3 = n_{31} - n_{32}i$. The index of refraction of the surface film is given by $\hat{n}_2 = n_{21} - n_{22}i$. The thickness of the surface film is given by d_2 . The following equations are used by the computer to calculate d_2 .

$$\hat{R}_n = \frac{\hat{r}_{12}^n + \hat{r}_{23}^n e^{\hat{s}}}{1 + \hat{r}_{12}^n \hat{r}_{23}^n e^{\hat{s}}} \quad (2.1)$$

$$\hat{R}_p = \frac{\hat{r}_{12}^p + \hat{r}_{23}^p e^{\hat{s}}}{1 + \hat{r}_{12}^p \hat{r}_{23}^p e^{\hat{s}}} \quad (2.2)$$

$$\hat{s} = \frac{-4\pi i}{\lambda} \cdot \hat{n}_2 \cos \hat{\phi}_2 d_2 \quad (2.3)$$

$$\frac{\hat{R}_p}{\hat{R}_n} = \tan \psi e^{i\Delta} \quad (2.4)$$

$$\hat{r}_{12}^n = \frac{n_1 \cos \phi_1 - \hat{n}_2 \cos \hat{\phi}_2}{n_1 \cos \phi_1 + \hat{n}_2 \cos \hat{\phi}_2} \quad (2.5)$$

(7) F. L. McCrackin and J. P. Colson, "A FORTRAN Program for Analysis of Ellipsometer Measurements and Calculations of Reflection Coefficients from Thin Films," Technical Note 242, U.S. Dept. of Commerce, Nat'l Bureau of Stds., Wash. D.C., 1964.

$$\hat{r}_{23}^n = \frac{\hat{n}_2 \cos \hat{\phi}_2 - \hat{n}_3 \cos \hat{\phi}_3}{\hat{n}_2 \cos \hat{\phi}_2 + \hat{n}_3 \cos \hat{\phi}_3} \quad (2.6)$$

$$\hat{r}_{12}^p = \frac{\hat{n}_2 \cos \phi_1 - n_1 \cos \hat{\phi}_2}{\hat{n}_2 \cos \phi_1 + n_1 \cos \hat{\phi}_2} \quad (2.7)$$

$$\hat{r}_{23}^p = \frac{\hat{n}_3 \cos \hat{\phi}_2 - \hat{n}_2 \cos \hat{\phi}_3}{\hat{n}_3 \cos \hat{\phi}_2 + \hat{n}_2 \cos \hat{\phi}_3} \quad (2.8)$$

$$\cos^2 \hat{\phi}_2 = 1 - \frac{n_1^2 \sin^2 \phi_1}{\hat{n}_2^2} \quad (2.9)$$

$$\cos^2 \hat{\phi}_3 = 1 - \frac{n_1^2 \sin^2 \phi_1}{\hat{n}_3^2} \quad (2.10)$$

n_1 = index of refraction of the surrounding medium.

ϕ_1 = angle of incidence.

λ = wavelength of the light beam.

$\hat{n}_3$ = index of refraction of the substrate.

$\hat{n}_2$ = index of refraction of the surface film.

d_2 = thickness of the surface film.

$\left. \begin{matrix} \psi \\ \Delta \end{matrix} \right\}$ = the experimental ellipsometric measurements.

Equation 2.1 and equation 2.2 are the exact Drude equations. Equation 2.4 is the fundamental ellipsometric equation. Equations 2.5 through 2.8 are the Fresnel reflection coefficients, and equation 2.9 and equation 2.10 were derived from Snell's Law.

Following the method of McCracking and Colson,⁽¹⁾ a complex quadratic equation is obtained of the form

$$\hat{A} e^{2\hat{s}} + \hat{B} e^{\hat{s}} + \hat{C} = 0 \quad (2.11)$$

by using equations 2.1, 2.2, and 2.4. Solving the quadratic equation for $e^{\hat{s}}$ and separating the real and imaginary terms, equation 2.11 reduces to the general form

$$e^{\hat{s}} = x + yi = \sqrt{x^2 + y^2} e^{i(\phi + 2n\pi)} \quad (2.12)$$

$$\text{where } \phi = \tan^{-1} y/x \text{ and} \quad (2.13)$$

$$n = 0, \pm 1, \pm 2, \dots$$

Taking the natural logarithm of both sides of equation 2.12 results in the equation

$$\hat{s} = \ln \sqrt{x^2 + y^2} + i(\phi + 2n\pi) \quad (2.14)$$

By equating equation 2.14 with equation 2.3, a complex equation for film thickness (d_2) can be obtained. There are two solutions for d_2 arising from the quadratic equation. The correct solution is chosen by selecting the value of d_2 with the smallest imaginary part. The real part is used as the thickness of the surface film.

3. Determining the Index of Refraction of the Surface Film

The index of refraction of the surface film is given by $\hat{n}_2 = n_{21} - n_{22}i$. The index of refraction is determined by first assuming a range of values for n_{22} . Then for a psi and delta measurement, a value of n_{22} is used with an iteration process to find a value for n_{21} which minimizes the imaginary part of film thickness. The process is repeated for all the psi and delta measurements in a set of data. The standard error* for the calculated n_{21} values is determined. The whole process is then repeated for the entire range assumed for n_{22} . The value of n_{22} which minimizes the standard error for n_{21} is selected as the imaginary part of $\hat{n}_2$ and the corresponding mean of the n_{21} calculations is selected as the real part of $\hat{n}_2$.

The iteration process for finding n_{21} is as follows. A range for n_{21} must be given and tested to determine if a solution for n_{21} exists in the given range. This is done by making film thickness calculations for a psi and delta ellipsometric measurement using the minimum and maximum values of the n_{21} range and the assumed value for n_{22} . The film thicknesses are, in general, complex. The signs of the two imaginary parts (minimum and maximum values of n_{21}) are compared. If the signs are the same, the range is too large or too small for a solution. If no solution exists, the next psi and delta measurement is processed. If the signs are opposite, there is a solution within the n_{21} range. To illustrate this point, a graph of the imaginary film thickness calculated for various values of n_{21} using $\psi = 30.70^\circ$,

$$* S_{\bar{y}} = \sqrt{\frac{\sum (X_i - \bar{X})^2}{n(n-1)}}$$

$\Delta = 114.15^\circ$, and $n_{22} = 1.5$ is presented in Figure 1. The values of psi and delta were calculated using $n_3 = 3.2 - 4.3i$, $\hat{n}_2 = 2.0 - 1.5i$ and $d_2 = 100\text{\AA}$.

Figure 2 shows the results using $\psi = 19.93^\circ$, $\Delta = 85.15^\circ$, and $n_{22} = 1.5$. These values for psi and delta were calculated using $d_2 = 1000\text{\AA}$. Note that in Figure 2, a second solution for n_{21} can be obtained, e.g., by specifying the n_{21} range to be 2.2–2.8. For the case where more than one solution exists, the correct solution will be the one having the maximum number of n_{21} values calculated for the set of psi and delta measurements.

A solution for n_{21} is desired which makes the imaginary part of film thickness approach zero. This can be conveniently done by calculating and comparing error terms for various values of n_{21} . An error term is determined by taking the film thickness calculated for the n_{21} value and using the real part to calculate psi and delta. The error term is defined by the equation

$$\epsilon = \sqrt{(\delta\psi)^2 + (\delta\Delta)^2}, \quad (3.1)$$

where $\delta\psi = \psi_{\text{experimental}} - \psi_{\text{calculated}}$ and
 $\delta\Delta = \Delta_{\text{experimental}} - \Delta_{\text{calculated}}$

This error criteria is used rather than the value of the imaginary part of the film thickness since ϵ relates directly to the quantities obtained from the ellipsometer and is therefore quantitatively more meaningful to the experiment. Upon testing for a solution for n_{21} , an error term is calculated at the midpoint of the n_{21} range. The half of the n_{21} range which contains the solution for n_{21} (as determined by the segment giving opposite signs of the imaginary part of film thickness) is selected. The half selected is again divided in half and another film thickness and error term are calculated. This process is repeated until a minimum error term is found.

A tolerance level can be used to aid the iteration process. Once the error term calculated is within the tolerance level specified, the iteration process for n_{21} terminates. The iteration process is limited by a given number of cycles. If a minimum error term or an error term within the tolerance level cannot be found within the number of cycles specified, a no solution criterion will be printed out by the computer.

Upon determining the index of refraction of the surface film, film thicknesses are computed for each of the psi and delta measurements.

FIGURE 1. Imaginary Film Thickness – versus – n_{21} for $\Psi = 30.70^\circ$ and $\Delta = 114.15^\circ$ for the Following Parameters: $n_1 = 1.00$, $\phi_1 = 70^\circ$, $\lambda = 5461\text{\AA}$, $\hat{n}_3 = 3.2 - 4.3i$ and $\hat{n}_2 = n_{21} - 1.5i$.

PROGRAM DESCRIPTION

The source program deck consists of a main program and seven subroutine subprograms (707 executable and non-executable statements, 798 cards). The memory requirements of the main program total 13,854 bytes and the memory requirements of the subroutine subprograms total 11,220 bytes. The source program deck can be compiled in four minutes and link edited in two minutes in an IBM S/360-40 computer. The execution time can be estimated from the number of psi and delta measurements processed. Film thicknesses are calculated and printed out in 0.4 second per psi, delta measurement. A line-printer output device with not less than 120 columns per line is sufficient for a print-out of results. A print-out of the source program is shown in Appendix A and an explanation of the FORTRAN IV notation is shown in Appendix B.

The source program consists of four parts, the computation and print-out of the index of refraction of the substrate material, the computation and print-out of the

thicknesses of the surface film, the determination of the index of refraction of the surface film followed by film thickness calculations, and the computation and print-out of the psi and delta optical parameters. Access to each part is controlled by the variable name IPICK as shown in Figure 3. Any or all of the four parts can be processed per run.

1. Computing the Index of Refraction of the Substrate Material

The index of refraction of the substrate material, $\hat{n}_3 = n_{31} - n_{32}i$, is calculated by the subroutine subprogram EN3. The calculations are direct and require:

- The index of refraction of the surrounding medium.
- The angle of incidence.
- The psi (ψ') and delta (Δ') measurements of the substrate material.

FIGURE 2. Imaginary Film Thickness - versus - n_{21} for $\Psi = 19.93^\circ$ and $\Delta = 85.15^\circ$ for the Following Parameters: $n_1 = 1.00$, $\phi_1 = 70^\circ$, $\lambda = 5461\text{\AA}$, $\hat{n}_3 = 3.2 - 4.3i$ and $\hat{n}_2 = n_{21} - 1.5i$.

FIGURE 3. Flowchart showing the Four Parts of the Source Program.

The input data can be punched into cards for a card read-punch input-output device. The data set has a title card and up to twenty measurements of psi and delta can be processed per run. Figure 4 shows the field format layout and gives a description of each of the cards.

The output data consist of the n_{31} and n_{32} values as shown in Figure 5.

2. Computing the Thickness of a Surface Film

The thickness of a surface film is calculated by the subroutine subprogram RID2. The calculations are direct and require:

- The index of refraction of the surrounding medium.
- The angle of incidence.
- The wavelength of the light beam.
- The index of refraction of the substrate.

e. The index of refraction of the surface film.

f. The experimental psi and delta measurements.

Part 2 of the program is useful when both the index of refraction of the substrate and the index of refraction of the surface film are known. The input data can be punched into cards for a card read-punch input-output device. The data set has a title card and up to thirty measurements of psi and delta can be processed per run. Figure 6 shows the field format layout and gives a description of each of the cards. The input data were obtained from F. L. McCrackin, Washington, D.C. in a private communication.

The growth of a surface film as measured by an ellipsometer can be described via the cycling of the angle phi (ϕ) in a rectilinear coordinate system. Phi is defined by equations 2.12 and 2.13.

$$e^{\delta} = x + yi = \sqrt{x^2 + y^2} e^{i(\phi + 2n\pi)} \quad (2.12)$$

$$\phi = \tan^{-1} y/x \quad (2.13)$$

$$n = 0, \pm 1, \pm 2,$$

FIGURE 4. Field Format Layout and Card Description of the Input Data for Part 1 of the Source Program.

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25
Card 1				0	4																				
Card 2				0	1																				
Card 3	0	D	A	T	A		S	E	T		N	O	.		1										
Card 4		1	.	0								7	0	.	0										
Card 5				0	1																				
Card 6	3	1	.	4	3							1	3	4	.	7	3								

Card 1 — The total number of data sets in the card deck.

Card 2 — The value of IPICK.

Card 3 — The title card (column 1 reserved for the digit 0 for carriage control).

Card 4 — The index of refraction of the surrounding medium and the angle of incidence in two 10-column fields, respectively.

Card 5 — The number of psi and delta measurements.

Card 6 — The psi and delta measurements in two 10-column fields, respectively, per card.

For an experimental set of psi and delta measurements of increasing film thickness, the angle phi cycles clockwise through the quadrants. To obtain the correct solution for film thickness d_2 , the value of n in equation 2.12 is -1 for the first cycle, -2 for the second cycle, etc. The growth of the film can be monitored by the computer by determining which quadrant phi is in from the values of x and y .

The subroutine subprogram QTEST2 determines the quadrant for the angle phi, corrects for the case where phi should fall in Quadrant III or Quadrant II,* and corrects for the complete cycling of phi. The subroutine subprogram QTEST is also used but strictly for placing phi in Quadrant III or Quadrant II.

The output data consist of the thickness of the surface film, the error term ϵ and the quadrant of the angle phi for each of the psi and delta measurements. The results of the test data are shown in Figure 7. The values of psi and delta for the film thicknesses from 0 to 1000Å in 100Å increments were calculated using the following parameters:

$$\begin{aligned} n_1 &= 1.0 \\ \phi_1 &= 70^\circ \\ \lambda &= 5461\text{Å} \\ \hat{n}_3 &= 3.2 - 4.3i \\ \hat{n}_2 &= 2.0 - 1.5i \end{aligned}$$

The calculated values for psi and delta were then rounded off to the second decimal place before being used in the calculations. Thus, small round-off errors will appear in the film thicknesses shown.

*The FORTRAN IV compiler will place phi in Quadrant I for the arctangent of a positive argument and in Quadrant IV for the arctangent of a negative argument.

3. Determining the Index of Refraction of the Surface Film and Computing Film Thickness

The index of refraction of the surface film, $\hat{n}_2 = n_{21} - n_{22}i$, is determined by the main program and the subroutine subprogram RID2. The main program calls in values of n_{22} , controls the iteration process for n_{21} , computes the error terms, and finally selects n_{21} and n_{22} for the index of refraction of the surface film. The subroutine subprogram RID2 calculates film thicknesses and values of psi and delta. The subroutine subprograms QTEST and QTEST3 correct and control the cycling of the angle phi. The latter subroutine subprogram is used especially for both the minimum and maximum values of the n_{21} range. The subroutine subprogram QTEST4 selects the quadrant for the optical parameter, delta (Δ), and the subroutine subprogram RANGE calculates values of n_{22} from a given range of n_{22} and the increment Δn_{22} .

In the main program, the iteration process for n_{21} uses three variable names, TOL, ITOL, and NTEST. The variable name TOL indicates a tolerance level of error which stops the cycling for n_{21} once the error term ϵ is within TOL. If ITOL=0, the value of TOL will be ignored and the computer could cycle NTEST times for n_{21} . If a solution is found, the error term ϵ is printed out along with the value of n_{21} computed for the psi and delta measurement. If n_{21} can't be determined in NTEST cycles, a no solution criterion is detected by the computer and the appropriate code number is printed out.

It is recommended that a tolerance level always be used but in the case where an appropriate tolerance level is not known, the computer can be used to determine one.

FIGURE 5. Output Data Showing the Results of Part 1 of the Source Program.

THE INDEX OF REFRACTION OF A CLEAN SURFACE DETERMINED BY THE METHOD OF ELLIPSOMETRY

DATA SET NO. 1

THE INDEX OF REFRACTION OF THE SURROUNDING MEDIUM IS 1.00
THE ANGLE OF INCIDENCE IS 70.00 DEGREES

	PSI PRIME	DEL PRIME	N31	N32
1	31.430	134.730	0.31999E 01	0.43012E 01

FIGURE 6. Field Format Layout and Card Description of the Input Data for Part 2 of the Source Program.

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25
Card 2				0	2																				
Card 3	0	D	A	T	A		S	E	T		N	O	.	2											
Card 4				1	.	0							7	0	.	0									
Card 5	5	4	6	1	.	0																			
Card 6				3	.	2								4	.	3									
Card 7				2	.	0								1	.	5									
Card 8				1	1																				
Card 9				3	1	.	4	3					1	3	4	.	7	3							
				3	0	.	7	0					1	1	4	.	1	5							
				2	9	.	3	6					9	9	.	8	9								
				2	7	.	6	1					9	0	.	1	3								
				2	5	.	6	3					8	3	.	7	6								
				2	3	.	6	4					8	0	.	3	3								
				2	1	.	9	4					7	9	.	4	7								
				2	0	.	7	6					8	0	.	4	2								
				2	0	.	1	2					8	2	.	1	6								
				1	9	.	9	0					8	3	.	8	8								
				1	9	.	9	3					8	5	.	1	5								

Card 2 — The value of IPICK.

Card 3 — The title card (column 1 reserved for the digit 0 for carriage control).

Card 4 — The index of refraction of the surrounding medium and the angle of incidence in two 10-column fields, respectively.

Card 5 — The wavelength of the light beam.

Card 6 — The real and imaginary parts of the refractive index of the substrate in two 10-column fields, respectively.

Card 7 — The real and imaginary parts of the refractive index of the surface film in two 10-column fields, respectively.

Card 8 — The number of psi and delta measurements.

Cards 9-19 — The psi and delta measurements in two 10-column fields, respectively, per card.

The input data for determining the index of refraction of the surface film consist of:

- a. The index of refraction of the surrounding medium.
- b. The angle of incidence.
- c. The wavelength of the light beam.
- d. The psi and delta measurements of the substrate material (IPICK = 3) or the real and imaginary parts of the refractive index of the substrate (IPICK=4).
- e. The minimum and maximum values of the n_{22} range with the increment Δn_{22} .
- f. The minimum and maximum values of the n_{21} range.
- g. The experimental psi and delta measurements.
- h. The tolerance level TOL for the set of data.

i. The value of ITOL.

j. The value of NTEST.

The input data can be punched into cards for a card read-punch input-output device. The data set has a title card and up to thirty measurements of psi and delta can be processed per run. Thirty values of n_{22} can also be processed per run. Figure 8 shows the field format layout and gives a description of each of the cards.

The output data consist of the values of n_{21} for the psi and delta measurements (or no solution at all), the error terms, the code numbers depicting the results of the iteration process and the mean value of n_{21} and the standard error for the set of data. A print-out will occur for each value of n_{22} used. Figure 9 shows the results for $n_{22} = 1.5$ which gives the minimum standard error for the mean of the n_{21} calculations and hence, the best index of refraction of the surface film. Figure 10 shows the resulting film thicknesses for $n_2 = 2.0-1.5i$.

FIGURE 7. Output Data Showing the Results of Part 2 of the Source Program.

THE THICKNESS OF A SURFACE FILM DETERMINED BY THE METHOD OF FILIPSOmetry

DATA SET NO. 2

THE INDEX OF REFRACTION OF THE SURROUNDING MEDIUM IS 1.00
 THE ANGLE OF INCIDENCE IS 70.00 DEGREES
 THE WAVELENGTH OF LIGHT IS 5461.00 ANGSTROMS
 THE INDEX OF REFRACTION OF THE SUBSTRATE IS N31 # 3.20 AND N32 # 4.30
 THE VALUE OF N21 IS 2.00
 THE VALUE OF N22 IS 1.50

	PSI	DELTA	THICKNESS	ERROR	QUADRANT
1	31.430	134.730	-0.2117979E-01	0.44336E-02	4
2	30.700	114.150	0.1000021E 03	0.56284E-02	4
3	29.360	99.890	0.2000097E 03	0.15028E-03	4
4	27.610	90.130	0.3000828E 03	0.36629E-02	4
5	25.630	83.760	0.4000750E 03	0.39866E-02	3
6	23.640	80.330	0.5001167E 03	0.47694E-03	3
7	21.940	79.470	0.6002280E 03	0.35722E-02	3
8	20.760	80.420	0.6998442E 03	0.25940E-02	3
9	20.120	82.160	0.7995803E 03	0.30755E-02	2
10	19.900	83.880	0.8998027E 03	0.21223E-02	2
11	19.930	85.150	0.9995212E 03	0.16854E-03	2

FIGURE 8. Field Format Layout and Card Description of the Input Data for Part 3 of the Source Program.

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25
Card 2			0	3																					
Card 3	0	D	A	T	A	S	E	T		N	O	.	3												
Card 4			1	.	0						7	0	.	0											
Card 5	5	4	6	1	.	0																			
Card 6			3	1	.	4	3				1	3	4	.	7	3									
Card 7			1	.	4	0					1	.	6	0					0	.	1				
Card 8			1	.	8						2	.	2												
Card 9			1	.	1																				
Card 10			3	1	.	4	3				1	3	4	.	7	3									
			3	0	.	7	0				1	1	4	.	1	5									
			2	9	.	3	6				9	9	.	8	9										
			2	7	.	6	1				9	0	.	1	3										
			2	5	.	6	3				8	3	.	7	6										
			2	3	.	6	4				8	0	.	3	3										
			2	1	.	9	4				7	9	.	4	7										
			2	0	.	7	6				8	0	.	4	2										
			2	0	.	1	2				8	2	.	1	6										
			1	9	.	9	0				8	3	.	8	8										
			1	9	.	9	3				8	5	.	1	5										
Card 21			0	.	0	1																			
Card 22			0	1																					
Card 23			1	0																					

Card 2 – The value of IPICK.

Card 3 – The title card (column 1 reserved for the digit 0 for carriage control).

Card 4 – The index of refraction of the surrounding medium and the angle of incidence in two 10-column fields, respectively.

Card 5 – The wavelength of the light beam.

Card 6 – The psi and delta measurements of the substrate material in two 10-column fields, respectively.

Card 7 – The minimum and maximum values of the n_{22} range and Δn_{22} in three 10-column fields, respectively.

Card 8 – The minimum and maximum values of the n_{21} range in two 10-column fields, respectively.

Card 9 – The number of psi and delta measurements.

Cards 10-20 – The psi and delta measurements in two 10-column fields, respectively, per card.

Card 21 – The tolerance level for the set of data.

Card 22 – The value of ITOL.

Card 23 – The value of NTEST.

THE OPTICAL CONSTANT N21 FOR PSI AND DELTA OR NO SOLUTION AT ALL
CALCULATING THE MEAN VALUE OF N21 FOR THE VALUE OF N22 USED

DATA SET NO. 3

THE INDEX OF REFRACTION OF THE SURROUNDING MEDIUM IS 1.00
THE ANGLE OF INCIDENCE IS 70.00 DEGREES
THE WAVELENGTH OF LIGHT IS 5461.00 ANGSTROMS
THE OPTICAL PARAMETERS OF THE SUBSTRATE ARE PSI PRIME # 31.430 AND DEL PRIME # 134.730
THE CALCULATED INDEX OF REFRACTION OF THE SUBSTRATE IS N31 # 0.31999E 01 AND N32 # 0.43012E 01
THE RANGE OF N22 IS MIN# 1.40, MAX# 1.60, DELTA# 0.10
THE RANGE OF N21 IS MIN# 1.80, MAX# 2.20
THE GIVEN TOLERANCE WHICH WAS EXECUTED IS 0.10000E-01, THE TEST VALUE IS 10
THE VALUE OF N22 IS 0.15000E 01

CODE 1 MEANS THE ABSOLUTE VALUE OF THE IMAGINARY THICKNESS IS LESS THAN OR EQUAL TO 0.1E-05 ANGSTROMS
CODE 3 MEANS THE GIVEN TOLERANCE WAS TOO SMALL IN SELECTING N21
CODE 4 MEANS THE GIVEN TOLERANCE WAS TOO LARGE IN SELECTING N21
CODE 5 MEANS THE GIVEN TOLERANCE WAS EXECUTED IN SELECTING N21
CODE 6 MEANS NO SOLUTION DUE TO LIKE SIGNS OF THE IMAGINARY PARTS OF FILM THICKNESS
CODE 7 MEANS NO SOLUTION, TOL TOO SMALL, TEST VALUE TOO SMALL, INCREASING ERROR IN COMPUTING N21
CODE 8 MEANS NO SOLUTION, TOL TOO SMALL, TEST VALUE TOO SMALL, DECREASING ERROR IN COMPUTING N21
CODE 9 MEANS NO SOLUTION, TOL TOO LARGE, TEST VALUE TOO SMALL, INCREASING ERROR IN COMPUTING N21
CODE 10 MEANS NO SOLUTION, TOL TOO LARGE, TEST VALUE TOO SMALL, DECREASING ERROR IN COMPUTING N21

	PSI	DELTA	N21	ERROR NOT EXCEEDING	CODE
1	31.430	134.730			6
2	30.700	114.150	0.1999999E 01	0.24232E-02	5
3	29.360	99.890	0.1999999E 01	0.26917E-02	5
4	27.610	90.130	0.1999999E 01	0.59493E-02	5
5	25.630	83.760	0.1999999E 01	0.63084E-02	5
6	23.640	80.330	0.1999999E 01	0.26845E-02	5
7	21.940	79.470			6
8	20.760	80.420			6
9	20.120	82.160	0.1999999E 01	0.36951E-02	5
10	19.900	83.880	0.1999999E 01	0.23747E-02	5
11	19.930	85.150	0.1999999E 01	0.12302E-03	5

THE MEAN VALUE OF N21 IS 0.1999999E 01, THE STANDARD ERROR FOR 8 VALUES OF N21 IS 0.0

FIGURE 9. Output Data showing the results leading to $\hat{n}_2 = 2.0 - 1.5i$, the Index of Refraction of the Surface Film for Part 3 of the Source Program.

4. Calculating the Psi and Delta Optical Parameters

Film thicknesses can be used to calculate psi and delta. Part 4 of the source program calculates the optical parameters for the film thicknesses given for any combination of n_{21} and n_{22} . The calculations are made by the subroutine subprogram RID2. The subroutine subprogram QTEST4 selects the quadrant for the optical parameter, delta (Δ). The subroutine subprogram RANGE calculates values of n_{22} and n_{21} from the minimum and maximum values of each of the given ranges. The ranges are incremented by Δn_{22} and Δn_{21} .

The main program consists of three DO loops. An innermost DO loop controls the given film thicknesses, a second DO loop controls the values of n_{21} and the third and outermost DO loop controls the values of n_{22} . The psi and delta optical parameters can be calculated for the film thicknesses for all of the n_{21} values for each of the n_{22} values.

The input data consist of:

- The index of refraction of the surrounding medium.
- The angle of incidence.
- The wavelength of the light beam.
- The index of refraction of the substrate.
- The minimum and maximum values of the n_{22} range with the increment Δn_{22} .
- The minimum and maximum values of the n_{21} range with the increment Δn_{21} .
- The film thicknesses.

FIGURE 10. Output Data Showing the Resulting Film Thicknesses for Part 3 of the Source Program.

THE THICKNESS OF A SURFACE FILM DETERMINED BY THE METHOD OF ELLIPSOMETRY

DATA SET NO. 3

THE INDEX OF REFRACTION OF THE SURROUNDING MEDIUM IS 1.00
 THE ANGLE OF INCIDENCE IS 70.00 DEGREES
 THE WAVELENGTH OF LIGHT IS 5461.00 ANGSTROMS
 THE INDEX OF REFRACTION OF THE SUBSTRATE IS N31 # 3.20 AND N32 # 4.30
 THE CALCULATED VALUE OF N21 IS 0.1999999E 01 WITH A STANDARD ERROR OF 0.0
 THE SELECTED VALUE OF N22 IS 0.15000E 01

	PSI	DELTA	THICKNESS	ERROR	QUADRANT
1	31.430	134.730	0.1980386E-03	0.48253E-04	1
2	30.700	114.150	0.1000234E 03	0.24232E-02	4
3	29.360	99.890	0.2000312E 03	0.26917E-02	4
4	27.610	90.130	0.3001042E 03	0.59493E-02	4
5	25.630	83.760	0.4000962E 03	0.63084E-02	3
6	23.640	80.330	0.5001365E 03	0.26845E-02	3
7	21.940	79.470	0.6002480E 03	0.17711E-02	3
8	20.760	80.420	0.6998682E 03	0.37578E-02	3
9	20.120	82.160	0.7996038E 03	0.36951E-02	2
10	19.900	83.880	0.8998267E 03	0.23747E-02	2
11	19.930	85.150	0.9995427E 03	0.12302E-03	2

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The input data can be punched into cards for a card read-punch input-output device. The data set has a title card and up to thirty values of film thickness can be processed per run. Thirty values each of n_{22} and n_{21} can also be processed per run. Figure 11 shows the field format layout and gives a description of each of the cards.

The output data consist of the psi and delta optical parameters. A print-out will occur for each combination of n_{21} and n_{22} . Figure 12 shows the results for the index of refraction of the surface film $\hat{n}_2 = 2.0 - 1.5i$.

FIGURE 11. Field Format Layout and Card Description of the Input Data for Part 4 of the Source Program.

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25
Card 2				0	5																				
Card 3	0	D	A	T	A		S	E	T		N	O	.	4											
Card 4				1	.	0							7	0	.	0									
Card 5	5	4	6	1	.	0																			
Card 6				3	.	2							4	.	3										
Card 7				1	.	4							1	.	6					0	.	1			
Card 8				1	.	9							2	.	1					0	.	1			
Card 9				1	1																				
Card 10				0	.	0							1	0	0	.	0								
				2	0	0	.	0					3	0	0	.	0								
				4	0	0	.	0					5	0	0	.	0								
				6	0	0	.	0					7	0	0	.	0								
				8	0	0	.	0					9	0	0	.	0								
				1	0	0	.	0																	

Card 2 – The value of IPICK.

Card 3 – The title card (column 1 reserved for the digit 0 for carriage control).

Card 4 – The index of refraction of the surrounding medium and the angle of incidence in two 10-column fields, respectively.

Card 5 – The wavelength of the light beam.

Card 6 – The real and imaginary parts of the refractive index of the substrate in two 10-column fields, respectively.

Card 7 – The minimum and maximum values of the n_{22} range and Δn_{22} in three 10-column fields, respectively.

Card 8 – The minimum and maximum values of the n_{21} range and Δn_{21} in three 10-column fields, respectively.

Card 9 – The number of values of film thickness.

Cards 10-15 – The film thicknesses in two 10-column fields per card.

FIGURE 12. Output Data Showing the Results of Part 4 of the Source Program.

THE OPTICAL PARAMETERS PSI AND DELTA DETERMINED BY THE METHOD OF ELLIPSOMETRY

DATA SET NO. 4

THE INDEX OF REFRACTION OF THE SURROUNDING MEDIUM IS 1.00
 THE ANGLE OF INCIDENCE IS 70.00 DEGREES
 THE WAVELENGTH OF LIGHT IS 5461.00 ANGSTROMS
 THE INDEX OF REFRACTION OF THE SUBSTRATE IS N31 # 3.20 AND N32 # 4.30
 THE RANGE OF N22 IS MIN# 1.40, MAX# 1.60, DELTA# 0.10
 THE RANGE OF N21 IS MIN# 1.90, MAX# 2.10, DELTA# 0.10
 THE VALUE OF N21 IS 2.00
 THE VALUE OF N22 IS 1.50

	THICKNESS	PSI CALC	DEL CALC
1	0.0	0.3142551E 02	0.1347252E 03
2	100.0	0.3069466E 02	0.1141520E 03
3	200.0	0.2936021E 02	0.9989101E 02
4	300.0	0.2761366E 02	0.9013362E 02
5	400.0	0.2563287E 02	0.8375986E 02
6	500.0	0.2364227E 02	0.8033186E 02
7	600.0	0.2194341E 02	0.7947301E 02
8	700.0	0.2075818E 02	0.8041972E 02
9	800.0	0.2011708E 02	0.8216476E 02
10	900.0	0.1989796E 02	0.8388197E 02
11	1000.0	0.1993053E 02	0.8515457E 02

APPENDIX A. Print-Out of the Source Program

Appendix A presents a complete print-out of the main program and the subroutine subprograms.

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C      001
C      A FORTRAN IV PROGRAM FOR COMPUTING THE THICKNESS OF A SURFACE 002
C      FILM AND DETERMINING ITS INDEX OF REFRACTION BY THE METHOD OF 003
C      ELLIPSOMETRY. 004
C      005
C      DIMENSION LABEL(18),PSIP(20),DELP(20),EN22(30),EN21(2),PSI(30) 006
C      DIMENSION DEL(30),D2(30),OPN21(30),NQ(30),D2I(2),ESUM(30) 007
C      DIMENSION ERROR(30),AVN21(30),SIGMA(30),K22(30),J21(30) 008
1      FORMAT(I5) 009
2      FORMAT(18A4) 010
3      FORMAT(2F10.3) 011
4      FORMAT(I5/(2F10.4)) 012
5      FORMAT('1THE INDEX OF REFRACTION OF A CLEAN SURFACE DETERMINED', 013
11X,'BY THE METHOD OF ELLIPSOMETRY') 014
6      FORMAT('0THE INDEX OF REFRACTION OF THE SURROUNDING MEDIUM IS', 015
11X,F5.2) 016
7      FORMAT(' THE ANGLE OF INCIDENCE IS',F6.2,1X,'DEGREES') 017
8      FORMAT('0',4X,'PSI PRIME',2X,'DEL PRIME',7X,'N31',13X,'N32'/) 018
9      FORMAT(1X,I2,4X,F6.3,4X,F7.3,3X,E12.5,4X,E12.5) 019
10     FORMAT(F10.4) 020
11     FORMAT(3F10.4) 021
12     FORMAT('1THE OPTICAL CONSTANT N21 FOR PSI AND DELTA OR NO', 022
11X,'SOLUTION AT ALL') 023
13     FORMAT(' CALCULATING THE MEAN VALUE OF N21 FOR THE VALUE', 024
11X,'OF N22 USED') 025
14     FORMAT(' THE WAVELENGTH OF LIGHT IS',F8.2,1X,'ANGSTROMS') 026
15     FORMAT(' THE OPTICAL PARAMETERS OF THE SUBSTRATE ARE PSI', 027
11X,'PRIME =',1X,F7.3,1X,'AND DEL PRIME =',1X,F8.3) 028
16     FORMAT(' THE CALCULATED INDEX OF REFRACTION OF THE SUBSTRATE IS', 029
11X,'N31 =',E12.5,1X,'AND N32 =',E12.5) 030
17     FORMAT(' THE INDEX OF REFRACTION OF THE SUBSTRATE IS', 031
11X,'N31 =',1X,F4.2,1X,'AND N32 =',1X,F4.2) 032
18     FORMAT(' THE RANGE OF N22 IS MIN=',F6.2,',',1X,'MAX=',F6.2,',', 033
11X,'DELTA=',F6.2) 034
19     FORMAT(' THE RANGE OF N21 IS MIN=',F6.2,',',1X,'MAX=',F6.2) 035
20     FORMAT(' THE GIVEN TOLERANCE WHICH WAS TESTED IS',E12.5,',',1X, 036
1'THE TEST VALUE IS',1X,I2) 037
21     FORMAT(' THE GIVEN TOLERANCE WHICH WAS EXECUTED IS',E12.5,',',1X, 038
1'THE TEST VALUE IS',1X,I2) 039
22     FORMAT(' THE VALUE OF N22 IS',E12.5) 040
23     FORMAT('CODE 1 MEANS THE ABSOLUTE VALUE OF THE IMAGINARY',1X, 041
1'THICKNESS IS LESS THAN OR EQUAL TO 0.1E-05 ANGSTROMS') 042
24     FORMAT(' CODE 2 MEANS THE GIVEN TOLERANCE WAS ADEQUATE IN',1X, 043
1'SELECTING N21') 044
25     FORMAT(' CODE 3 MEANS THE GIVEN TOLERANCE WAS TOO SMALL IN',1X, 045
1'SELECTING N21') 046
26     FORMAT(' CODE 4 MEANS THE GIVEN TOLERANCE WAS TOO LARGE IN',1X, 047
1'SELECTING N21') 048
27     FORMAT(' CODE 5 MEANS THE GIVEN TOLERANCE WAS EXECUTED IN',1X, 049
1'SELECTING N21') 050
28     FORMAT(' CODE 6 MEANS NO SOLUTION DUE TO LIKE SIGNS OF THE',1X, 051
1'IMAGINARY PARTS OF FILM THICKNESS') 052
29     FORMAT(' CODE 7 MEANS NO SOLUTION, TOL TOO SMALL, TEST VALUE',1X, 053
1'TOO SMALL, INCREASING ERROR IN COMPUTING N21') 054
30     FORMAT(' CODE 8 MEANS NO SOLUTION, TOL TOO SMALL, TEST VALUE',1X, 055
1'TOO SMALL, DECREASING ERROR IN COMPUTING N21') 056
31     FORMAT(' CODE 9 MEANS NO SOLUTION, TOL TOO LARGE, TEST VALUE',1X, 057
1'TOO LARGE, DECREASING ERROR IN COMPUTING N21') 058

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1'TOO SMALL, INCREASING ERROR IN COMPUTING N21')          059
32  FORMAT(' CODE 10 MEANS NO SOLUTION, TOL TOO LARGE, TEST VALUE', 060
11X,'TOO SMALL, DECREASING ERROR IN COMPUTING N21')        061
33  FORMAT('0',6X,'PSI',6X,'DELTA',10X,'N21',7X,'ERROR NOT EXCEEDING',062
12X,'CODE'/)                                               063
34  FORMAT(1X,I2,3X,F6.3,3X,F7.3,41X,I1)                  064
35  FORMAT(1X,I2,3X,F6.3,3X,F7.3,3X,E14.7,5X,E12.5,7X,I1) 065
36  FORMAT('0THE MEAN VALUE OF N21 IS',E14.7,', THE STANDARD ERROR', 066
11X,'FOR',1X,I2,' VALUES OF N21 IS',E14.7)              067
37  FORMAT('1THE THICKNESS OF A SURFACE FILM DETERMINED BY THE', 068
11X,'METHOD OF ELLIPSOMETRY')                              069
38  FORMAT(' THE VALUE OF N21 IS',1X,F5.2)                 070
39  FORMAT(' THE VALUE OF N22 IS',1X,F5.2)                 071
40  FORMAT(' THE CALCULATED VALUE OF N21 IS',E14.7,1X,      072
1'WITH A STANDARD ERROR OF',E12.5)                        073
41  FORMAT(' THE SELECTED VALUE OF N22 IS',                 074
11X,E12.5)                                                  075
42  FORMAT('0',6X,'PSI',6X,'DELTA',7X,'THICKNESS',9X,'ERROR', 076
13X,'QUADRANT'/)                                           077
43  FORMAT(1X,I2,3X,F6.3,3X,F7.3,3X,E14.7,3X,E12.5,3X,I1) 078
44  FORMAT('1THE OPTICAL PARAMETERS PSI AND DELTA DETERMINED BY THE', 079
11X,'METHOD OF ELLIPSOMETRY')                              080
45  FORMAT(' THE RANGE OF N21 IS MIN=',F6.2,',',1X,'MAX=',F6.2,',', 081
11X,'DELTA=',F6.2)                                         082
46  FORMAT('0',4X,'THICKNESS',4X,'PSI CALC',9X,'DEL CALC'/) 083
47  FORMAT(1X,I2,3X,F6.1,3X,E14.7,3X,E14.7)               084
    JJ=1                                                    085
    KK=3                                                    086
C                                                            087
C  COMPUTING THE INDEX OF REFRACTION OF A CLEAN SURFACE.  088
C  WRITING THE RESULTS.                                    089
C                                                            090
C  READING AND DERIVING INPUT DATA.                       091
C                                                            092
    READ(JJ,1)NUMBER                                       093
    DO 200 KRET=1,NUMBER                                    094
    READ(JJ,1)IPICK                                         095
    GO TO (1005,1010,1015,1015,1020),IPICK                096
1005 READ(JJ,2)LABEL                                       097
    READ(JJ,3)EN1,PHI1                                       098
    READ(JJ,4)NSETS,(PSIP(J),DELP(J),J=1,NSETS)           099
    WRITE(KK,5)                                              100
    WRITE(KK,2)LABEL                                         101
    WRITE(KK,6)EN1                                           102
    WRITE(KK,7)PHI1                                          103
    WRITE(KK,8)                                              104
    EN31=0.0                                                 105
    EN32=0.0                                                 106
    DO 205 J=1,NSETS                                         107
    CALL EN3(EN1,PHI1,PSIP(J),DELP(J),EN31,EN32)          108
    WRITE(KK,9)J,PSIP(J),DELP(J),EN31,EN32                109
205  CONTINUE                                              110
    GO TO 200                                                111
1010 READ(JJ,2)LABEL                                       112
    READ(JJ,3)EN1,PHI1                                       113
    READ(JJ,10)WAVE                                          114
    READ(JJ,3)EN31,EN32                                       115
    READ(JJ,3)EN21(1),EN22(1)                               116

```

	READ(JJ,4)NSETS,(PSI(J),DEL(J),J=1,NSETS)	117
	GO TO 1025	118
1015	READ(JJ,2)LABEL	119
	READ(JJ,3)EN1,PHI1	120
	READ(JJ,10)WAVE	121
	IF(IPICK-4)50,51,51	122
51	READ(JJ,3)EN31,EN32	123
	GO TO 1030	124
50	READ(JJ,3)PSIP(1),DELP(1)	125
	EN31=0.0	126
	EN32=0.0	127
	CALL EN3(EN1,PHI1,PSIP(1),DELP(1),EN31,EN32)	128
1030	READ(JJ,11)EN22N,EN22X,DN22	129
	READ(JJ,3)EN21N,EN21X	130
	READ(JJ,4)NSETS,(PSI(J),DEL(J),J=1,NSETS)	131
	READ(JJ,10)TOL	132
	READ(JJ,1)ITOL	133
	READ(JJ,1)NTEST	134
	DO 210 K=1,30	135
	EN22(K)=0.0	136
210	CONTINUE	137
	N22=0	138
	CALL RANGE(EN22N,EN22X,DN22,N22,EN22)	139
	GO TO 1035	140
1020	READ(JJ,2)LABEL	141
	READ(JJ,3)EN1,PHI1	142
	READ(JJ,10)WAVE	143
	READ(JJ,3)EN31,EN32	144
	READ(JJ,11)EN22N,EN22X,DN22	145
	READ(JJ,11)EN21N,EN21X,DN21	146
	READ(JJ,4)NSETS,(D2(J),J=1,NSETS)	147
	DO 215 K=1,30	148
	EN22(K)=0.0	149
	OPN21(K)=0.0	150
215	CONTINUE	151
	N22=0	152
	CALL RANGE(EN22N,EN22X,DN22,N22,EN22)	153
	N21=0	154
	CALL RANGE(EN21N,EN21X,DN21,N21,OPN21)	155
	GO TO 1040	156
C		157
C	DETERMINING THE INDEX OF REFRACTION OF THE SURFACE FILM.	158
C		159
1035	DO 220 K=1,N22	160
	DO 225 J=1,NSETS	161
	D2(J)=0.0	162
	NQ(J)=0	163
225	CONTINUE	164
	D2I(1)=0.0	165
	RADS=0.0	166
	LS=0	167
	RADD=0.0	168
	LD=0	169
	CYCLES=0.0	170
	JC1S=0	171
	JC2S=0	172
	KCS=0	173
	LCS=0	174

CYCLED=0.0	175
JC1D=0	176
JC2D=0	177
KCD=0	178
LCD=0	179
DO 230 J=1,NSETS	180
MCS=0	181
MCD=0	182
EN21(1)=EN21N	183
EN21(2)=EN21X	184
PSIC=0.0	185
DELC=0.0	186
IPATH=1	187
I=1	188
ISHIFT=1	189
NTOL=NTEST+1	190
IVARI=0	191
JVARI=0	192
KVARI=0	193
LVARI=0	194
L=1	195
1050 D2I(2)=0.0	196
CALL RID2(EN22(K),PSI(J),DEL(J),EN21(I),ISHIFT,D2(J),NQ(J),D2I(I),	197
1PSIC,DELC,EN31,EN32,EN1,PHI1,WAVE,RADS,LS,RADD,LD,CYCLES,I,JC1S,	198
2JC2S,KCS,LCS,MCS,CYCLED,JC1D,JC2D,KCD,LCD,MCD,J,IPICK)	199
RADS=CYCLES	200
RADD=CYCLED	201
IF(ABS(D2I(1))-0.1E-05)52,52,53	202
52 OPN21(J)=EN21(I)	203
IDIAG=1	204
ERROR(J)=0.0	205
GO TO 1045	206
53 IF(IPATH-2)54,55,55	207
54 IPATH=2	208
I=2	209
GO TO 1050	210
55 IF(D2I(1))56,56,57	211
56 IF(D2I(2))58,58,59	212
57 IF(D2I(2))59,59,58	213
58 IF(IPATH-3)60,61,61	214
60 IDIAG=6	215
GO TO 1045	216
59 IF(IPATH-3)62,63,63	217
62 IPATH=3	218
ISHIFT=2	219
1055 AVE1=(EN21(1)+EN21(2))/2.0	220
AVE2=EN21(2)	221
EN21(2)=AVE1	222
GO TO 1050	223
61 D2I(1)=D2I(2)	224
EN21(1)=AVE1	225
EN21(2)=AVE2	226
63 EPSI=PSI(J)-PSIC	227
EDEL=DEL(J)-DELC	228
ESUM(L)=SQRT(EPSI**2+EDEL**2)	229
IF(ESUM(L)-TOL)64,64,65	230
64 IF(ITOL)66,66,67	231
67 OPN21(J)=AVE1	232

	ERROR(J)=ESUM(L)	233
	IDIAG=5	234
	GO TO 1045	235
66	KVARI=KVARI+1	236
	NTOL=L	237
65	IF(L-2)68,69,69	238
68	L=L+1	239
	GO TO 1055	240
69	IF(KVARI-L)70,71,71	241
71	LVARI=1	242
	GO TO 1060	243
70	IF(NTOL-L)72,73,1060	244
72	ESUM(1)=ESUM(L-1)	245
	ERROR(J)=ESUM(1)	246
	IDIAG=2	247
	GO TO 1065	248
73	ESUM(1)=ESUM(L)	249
	ERROR(J)=ESUM(1)	250
	IDIAG=2	251
	GO TO 1065	252
1060	IF(ESUM(L)-ESUM(L-1))74,74,75	253
75	JVARI=1	254
	IF(IVARI)76,76,77	255
77	ESUM(1)=ESUM(L-1)	256
1070	ERROR(J)=ESUM(1)	257
	IF(LVARI)78,78,79	258
78	IDIAG=3	259
	GO TO 1065	260
79	IDIAG=4	261
	GO TO 1065	262
74	IVARI=1	263
	IF(JVARI)76,76,80	264
80	ESUM(1)=ESUM(L)	265
	GO TO 1070	266
76	IF(L-NTTEST)81,82,82	267
81	L=L+1	268
	GO TO 1055	269
82	IF(KVARI-L)83,84,84	270
84	IF(IVARI)85,85,86	271
86	IDIAG=10	272
	GO TO 1045	273
85	IDIAG=9	274
	GO TO 1045	275
83	IF(IVARI)87,87,88	276
88	IDIAG=8	277
	GO TO 1045	278
87	IDIAG=7	279
	GO TO 1045	280
1065	AVEP=(EN21(1)+EN21(2))/2.0	281
	AVE2=EN21(2)	282
	EN21(2)=AVEP	283
	AVEL=(EN21(1)+AVEP)/2.0	284
	AVER=(AVEP+AVE2)/2.0	285
	DO 235 L=2,3	286
	D2I(2)=0.0	287
	CALL RID2(EN22(K),PSI(J),DEL(J),EN21(2),ISHIFT,D2(J),NQ(J),D2I(2),	288
	1PSIC,DELC,EN31,EN32,EN1,PHI1,WAVE,RADS,LS,RADD,LD,CYCLES,I,JC1S,	289
	2JC2S,KCS,LCS,MCS,CYCLED,JC1D,JC2D,KCD,LCD,MCD,J,IPICK)	290

	EPSI=PSI(J)-PSIC	291
	EDEL=DEL(J)-DELC	292
	ESUM(L)=SQRT(EPSI**2+EDEL**2)	293
	IF(L-3)89,90,90	294
89	IF(D2I(1))91,91,92	295
91	IF(D2I(2))93,93,94	296
92	IF(D2I(2))94,94,93	297
93	AVE=AVER	298
	OPN21(J)=AVE2	299
	IF(ESUM(L)-ESUM(1))95,95,96	300
95	EN21(2)=(AVEP+AVE)/2.0	301
	MVARI=1	302
	GO TO 235	303
96	EN21(2)=(AVE+AVE2)/2.0	304
	MVARI=0	305
	GO TO 235	306
94	AVE=AVEL	307
	OPN21(J)=EN21(1)	308
	IF(ESUM(L)-ESUM(1))95,95,97	309
97	EN21(2)=(EN21(1)+AVE)/2.0	310
	MVARI=0	311
	GO TO 235	312
90	IF(MVARI)98,98,99	313
99	IF(ESUM(L)-ESUM(2))100,100,101	314
101	OPN21(J)=AVEP	315
	GO TO 235	316
98	IF(ESUM(L)-ESUM(1))100,100,235	317
100	OPN21(J)=EN21(2)	318
235	CONTINUE	319
C		320
C	WRITING THE OPTICAL CONSTANT N21 FOR PSI AND DELTA.	321
C		322
1045	IF(J-2)102,103,103	323
102	WRITE(KK,12)	324
	WRITE(KK,13)	325
	WRITE(KK,2)LABEL	326
	WRITE(KK,6)EN1	327
	WRITE(KK,7)PHI1	328
	WRITE(KK,14)WAVE	329
	IF(IPICK-4)104,105,105	330
104	WRITE(KK,15)PSIP(1),DELP(1)	331
	WRITE(KK,16)EN31,EN32	332
	GO TO 1075	333
105	WRITE(KK,17)EN31,EN32	334
1075	WRITE(KK,18)EN22N,EN22X,DN22	335
	WRITE(KK,19)EN21N,EN21X	336
	IF(ITOL)106,106,107	337
106	WRITE(KK,20)TOL,NTEST	338
	NJ=1	339
	GO TO 1080	340
107	WRITE(KK,21)TOL,NTEST	341
	NJ=2	342
1080	WRITE(KK,22)EN22(K)	343
	WRITE(KK,23)	344
	GO TO (1085,1090),NJ	345
1085	WRITE(KK,24)	346
1090	WRITE(KK,25)	347
	WRITE(KK,26)	348

	IF(ITOL)108,108,109	349
109	WRITE(KK,27)	350
108	WRITE(KK,28)	351
	WRITE(KK,29)	352
	WRITE(KK,30)	353
	WRITE(KK,31)	354
	WRITE(KK,32)	355
	WRITE(KK,33)	356
103	IF(IDIAG-6)110,111,111	357
111	WRITE(KK,34)J,PSI(J),DEL(J),IDIAG	358
	J21(J)=0	359
	GO TO 230	360
110	WRITE(KK,35)J,PSI(J),DEL(J),OPN21(J),ERROR(J),IDIAG	361
	J21(J)=1	362
230	CONTINUE	363
C		364
C	APPROXIMATING THE OPTICAL CONSTANT N21 OF THE SURFACE FILM.	365
C		366
	ICOUNT=0	367
	DO 240 J=1,NSETS	368
	IF(J21(J))240,240,112	369
112	ICOUNT=ICOUNT+1	370
240	CONTINUE	371
	IF(ICOUNT-2)113,114,114	372
113	K22(K)=0	373
	GO TO 220	374
114	SUM1=0.0	375
	SUM2=0.0	376
	DO 245 J=1,NSETS	377
	IF(J21(J))245,245,115	378
115	SUM1=SUM1+OPN21(J)	379
	SUM2=SUM2+OPN21(J)**2	380
245	CONTINUE	381
	ANSETS=ICOUNT	382
	AVN21(K)=SUM1/ANSETS	383
	SUM1=(SUM1**2)/ANSETS	384
	IF(SUM2-SUM1)116,117,117	385
116	SIGMA(K)=0.0	386
	GO TO 1095	387
117	SIGMA(K)=SQRT((SUM2-SUM1)/((ANSETS-1.0)*ANSETS))	388
1095	WRITE(KK,36)AVN21(K),ICOUNT,SIGMA(K)	389
	K22(K)=1	390
220	CONTINUE	391
C		392
C	SELECTING THE OPTICAL CONSTANT N22 OF THE SURFACE FILM.	393
C		394
	DO 250 K=1,N22	395
	IF(K22(K))250,250,118	396
250	CONTINUE	397
	GO TO 200	398
118	IF(K-N22)119,120,120	399
119	L=K+1	400
	DO 255 I=L,N22	401
	IF(K22(I))255,255,121	402
121	IF(SIGMA(K)-SIGMA(I))255,255,122	403
122	K=I	404
255	CONTINUE	405
120	EN21(1)=AVN21(K)	406

	SIGMA(1)=SIGMA(K)	407
	EN22(1)=EN22(K)	408
C		409
C	COMPUTING THE THICKNESS OF THE SURFACE FILM. WRITING THE RESULTS.	410
C		411
1025	DO 260 J=1,NSETS	412
	D2(J)=0.0	413
	NQ(J)=0	414
260	CONTINUE	415
	PSIC=0.0	416
	DELC=0.0	417
	RADS=0.0	418
	LS=0	419
	RADD=0.0	420
	LD=0	421
	CYCLES=0.0	422
	I=0	423
	JC1S=0	424
	JC2S=0	425
	KCS=0	426
	LCS=0	427
	MCS=0	428
	CYCLED=0.0	429
	JC1D=0	430
	JC2D=0	431
	KCD=0	432
	LCD=0	433
	MCD=0	434
	IPICK2=2	435
	ISHIFT=2	436
	DO 265 J=1,NSETS	437
	D2I(1)=0.0	438
	CALL RID2(EN22(1),PSI(J),DEL(J),EN21(1),ISHIFT,D2(J),NQ(J),D2I(1),	439
	1PSIC,DELC,EN31,EN32,EN1,PHI1,WAVE,RADS,LS,RADD,LD,CYCLES,I,JC1S,	440
	2JC2S,KCS,LCS,MCS,CYCLED,JC1D,JC2D,KCD,LCD,MCD,J,IPICK2)	441
	EPSI=PSI(J)-PSIC	442
	EDEL=DEL(J)-DELC	443
	ESUM(J)=SQRT(EPSI**2+EDEL**2)	444
	ISHIFT=3	445
265	CONTINUE	446
	WRITE(KK,37)	447
	WRITE(KK,2) LABEL	448
	WRITE(KK,6) EN1	449
	WRITE(KK,7) PHI1	450
	WRITE(KK,14) WAVE	451
	WRITE(KK,17) EN31, EN32	452
	IF(IPICK-2) 123,123,124	453
123	WRITE(KK,38) EN21(1)	454
	WRITE(KK,39) EN22(1)	455
	GO TO 1100	456
124	WRITE(KK,40) EN21(1),SIGMA(1)	457
	WRITE(KK,41) EN22(1)	458
1100	WRITE(KK,42)	459
	WRITE(KK,43) (J,PSI(J),DEL(J),D2(J),ESUM(J),NQ(J),J=1,NSETS)	460
	GO TO 200	461
C		462
C	CALCULATING THE OPTICAL PARAMETERS PSI AND DELTA FROM THE	463
C	THICKNESS OF THE SURFACE FILM. WRITING THE RESULTS.	464

C		465
1040	DO 270 J=1,NSETS	466
	PSI(J)=0.0	467
	DEL(J)=0.0	468
	NQ(J)=0	469
270	CONTINUE	470
	D2I(1)=0.0	471
	PSIC=0.0	472
	DELC=0.0	473
	RADS=0.0	474
	LS=0	475
	RADD=0.0	476
	LD=0	477
	CYCLES=0.0	478
	IC=0	479
	JC1S=0	480
	JC2S=0	481
	KCS=0	482
	LCS=0	483
	MCS=0	484
	CYCLED=0.0	485
	JC1D=0	486
	JC2D=0	487
	KCD=0	488
	LCD=0	489
	MCD=0	490
	DO 275 K=1,N22	491
	DO 280 I=1,N21	492
	WRITE(KK,44)	493
	WRITE(KK,2) LABEL	494
	WRITE(KK,6) EN1	495
	WRITE(KK,7) PHI1	496
	WRITE(KK,14) WAVE	497
	WRITE(KK,17) EN31, EN32	498
	WRITE(KK,18) EN22N, EN22X, DN22	499
	WRITE(KK,45) EN21N, EN21X, DN21	500
	WRITE(KK,38) OPN21(I)	501
	WRITE(KK,39) EN22(K)	502
	WRITE(KK,46)	503
	ISHIFT=4	504
	DO 285 J=1,NSETS	505
	CALL RID2(EN22(K),PSI(J),DEL(J),OPN21(I),ISHIFT,D2(J),NQ(J),	506
	1D2I(1),PSIC,DELC,EN31,EN32,EN1,PHI1,WAVE,RADS,LS,RADD,LD,CYCLES,	507
	2IC,JC1S,JC2S,KCS,LCS,MCS,CYCLED,JC1D,JC2D,KCD,LCD,MCD,J,IPICK)	508
	WRITE(KK,47) J,D2(J),PSIC,DELC	509
	ISHIFT=5	510
285	CONTINUE	511
280	CONTINUE	512
275	CONTINUE	513
200	CONTINUE	514
	STOP	515
	END	516
	SUBROUTINE EN3(EN1,PHI1,PSIP,DELP,EN31,EN32)	517
	SPHI=SIN(PHI1/57.29578)	518
	CPhi=cos(PHI1/57.29578)	519
	SPSI=SIN(2.0*PSIP/57.29578)	520
	CPSI=cos(2.0*PSIP/57.29578)**2	521
	SDEL=SIN(DELP/57.29578)	522

	CDEL=COS(DELP/57.29578)	523
	T=SPHI/CPHI	524
	AV=T*T*CPSI/((1.0+SPSI*CDEL)**2)	525
	A1=EN1**2*SPHI**2*(1.0+AV)	526
	A2=EN1*T*SPHI*SPSI*SDEL/(1.0+SPSI*CDEL)	527
	A=A1-A2**2	528
	A3=(A1-EN1**2*SPHI**2)/A1	529
	B=2.0*A2*SQRT(A1*A3)	530
	S=SQRT(A*A+B*B)	531
	EN31=SQRT((S+A)/2.0)	532
	EN32=SQRT((S-A)/2.0)	533
	RETURN	534
	END	535
	SUBROUTINE RANGE(ENI,ENF,DELTA,N,EN)	536
	DIMENSION EN(30)	537
	P=(ENF-ENI)/DELTA+1.1	538
	EN(1)=ENI	539
	N=P	540
	IF(N-1)2,2,4	541
4	DO 100 I=2,N	542
	EN(I)=EN(I-1)+DELTA	543
100	CONTINUE	544
2	RETURN	545
	END	546
	SUBROUTINE RID2(EN22,PSI,DEL,EN21,ISHIFT,D2,NQ,D2I,PSIC,DELC,	547
	1EN31,EN32,EN1,PHI1,WAVE,RADS,LS,RADD,LD,CYCLES,IC,JC1S,JC2S,	548
	2KCS,LCS,MCS,CYCLED,JC1D,JC2D,KCD,LCD,MCD,J,IPICK)	549
C		550
C	CALCULATING FILM THICKNESS D2.	551
C		552
	GO TO (2,2,4,2,8),ISHIFT	553
2	APH=COS(PHI1/57.29578)	554
	APHS=APH*APH	555
	A1=EN1*EN1	556
	A31=EN31*EN31	557
	A32=EN32*EN32	558
	A11=A31+A32	559
	AG3=1.0-(A1*A31-A1*A32+APHS*(A1*A32-A1*A31))/(A11*A11)	560
	AH3=(2.0*A1*EN31*EN32*(1.0-APHS))/(A11*A11)	561
	ARH03=0.0	562
	CALL QTEST(AH3,AG3,ARH03)	563
	ARH03=ARH03*0.5	564
	A2=(AG3*AG3+AH3*AH3)**0.25	565
	AI3=A2*COS(ARH03)	566
	AJ3=A2*SIN(ARH03)	567
	A21=EN21*EN21	568
	A22=EN22*EN22	569
	A12=A21+A22	570
	AG2=1.0-(A1*A21-A1*A22+APHS*(A1*A22-A1*A21))/(A12*A12)	571
	AH2=(2.0*A1*EN21*EN22*(1.0-APHS))/(A12*A12)	572
	ARH02=0.0	573
	CALL QTEST(AH2,AG2,ARH02)	574
	ARH02=ARH02*0.5	575
	A2=(AG2*AG2+AH2*AH2)**0.25	576
	AI2=A2*COS(ARH02)	577
	AJ2=A2*SIN(ARH02)	578
	AU=EN21*AJ2+EN22*AI2	579
	AV=EN21*AI2-EN22*AJ2	580

	A1=AU*AU+AV*AV	581
	A2=-WAVE/(4.0*3.141593)	582
	AP2=AU/A2	583
	BP2=AV/A2	584
C		585
	B1N12=EN1*APH-EN21*AI2+EN22*AJ2	586
	B2N12=EN1*APH+EN21*AI2-EN22*AJ2	587
	B3N12=EN21*AJ2+EN22*AI2	588
	B1P12=EN21*APH-EN1*AI2	589
	B2P12=EN22*APH-EN1*AJ2	590
	B3P12=EN21*APH+EN1*AI2	591
	B4P12=EN22*APH+EN1*AJ2	592
	B1N23=EN21*AI2-EN22*AJ2-EN31*AI3+EN32*AJ3	593
	B2N23=EN21*AI2-EN22*AJ2+EN31*AI3-EN32*AJ3	594
	B3N23=EN31*AJ3+EN32*AI3-EN21*AJ2-EN22*AI2	595
	B4N23=EN31*AJ3+EN32*AI3+EN21*AJ2+EN22*AI2	596
	B1P23=EN31*AI2-EN32*AJ2-EN21*AI3+EN22*AJ3	597
	B2P23=EN31*AI2-EN32*AJ2+EN21*AI3-EN22*AJ3	598
	B3P23=EN21*AJ3+EN22*AI3-EN31*AJ2-EN32*AI2	599
	B4P23=EN21*AJ3+EN22*AI3+EN31*AJ2+EN32*AI2	600
C		601
	C1=(B1N12*B2N12-B3N12*B3N12)/(B2N12*B2N12+B3N12*B3N12)	602
	C2=(B1N12*B3N12+B3N12*B2N12)/(B2N12*B2N12+B3N12*B3N12)	603
	C3=(B1P12*B3P12+B2P12*B4P12)/(B3P12*B3P12+B4P12*B4P12)	604
	C4=(B1P12*B4P12-B2P12*B3P12)/(B3P12*B3P12+B4P12*B4P12)	605
	C5=(B1N23*B2N23-B3N23*B4N23)/(B2N23*B2N23+B4N23*B4N23)	606
	C6=(B1N23*B4N23+B3N23*B2N23)/(B2N23*B2N23+B4N23*B4N23)	607
	C7=(B1P23*B2P23-B3P23*B4P23)/(B2P23*B2P23+B4P23*B4P23)	608
	C8=(B1P23*B4P23+B3P23*B2P23)/(B2P23*B2P23+B4P23*B4P23)	609
	GO TO (4,4,8,8), ISHIFT	610
C		611
4		612
	CPSI=COS(PSI/57.29578)	613
	SPSI=SIN(PSI/57.29578)	614
	TP=SPSI/CPSI	615
	SD=SIN(DEL/57.29578)	616
	CD=COS(DEL/57.29578)	617
	AQ1=C3*C5*C7*CD*TP-C4*C5*C7*SD*TP-C3*C5*C8*SD*TP-C4*C5*C8*CD*TP	618
	1-C3*C6*C7*SD*TP-C4*C6*C7*CD*TP-C3*C6*C8*CD*TP+C4*C6*C8*SD*TP	619
	2-C1*C5*C7+C1*C6*C8+C2*C6*C7+C2*C5*C8	620
	AQ2=C3*C5*C7*SD*TP+C4*C5*C7*CD*TP+C3*C5*C8*CD*TP+C3*C6*C7*CD*TP	621
	1-C4*C5*C8*SD*TP-C4*C6*C7*SD*TP-C3*C6*C8*SD*TP-C4*C6*C8*CD*TP	622
	2+C2*C6*C8-C2*C5*C7-C1*C5*C8-C1*C6*C7	623
	BQ1=C5*CD*TP-C6*SD*TP+C1*C3*C7*CD*TP-C1*C4*C8*CD*TP	624
	1-C2*C3*C8*CD*TP-C2*C4*C7*CD*TP-C1*C3*C8*SD*TP-C1*C4*C7*SD*TP	625
	2-C2*C3*C7*SD*TP+C2*C4*C8*SD*TP-C1*C3*C5+C2*C4*C5+C2*C3*C6	626
	3+C1*C4*C6-C7	627
	BQ2=C6*CD*TP+C5*SD*TP+C1*C3*C8*CD*TP+C1*C4*C7*CD*TP	628
	1+C2*C3*C7*CD*TP-C2*C4*C8*CD*TP+C1*C3*C7*SD*TP-C1*C4*C8*SD*TP	629
	2-C2*C3*C8*SD*TP-C2*C4*C7*SD*TP-C2*C3*C5-C1*C4*C5-C1*C3*C6	630
	3+C2*C4*C6-C8	631
	CQ1=C1*CD*TP-C2*SD*TP-C3	632
	CQ2=C2*CD*TP+C1*SD*TP-C4	633
C		634
	EA=BQ1*BQ1-BQ2*BQ2-4.0*AQ1*CQ1+4.0*AQ2*CQ2	635
	EB=2.0*BQ1*BQ2-4.0*AQ1*CQ2-4.0*AQ2*CQ1	636
	ERH01=0.0	637
	CALL QTEST(EB,EA,ERH01)	638
	ERH01=ERH01*0.5	

```

E1=(EA*EA+EB*EB)**0.25 639
E2=2.0*(AQ1*AQ1+AQ2*AQ2) 640
ERHO2=E1*(AQ1*COS(ERHO1)+AQ2*SIN(ERHO1)) 641
XSUM=(-AQ1*BQ1-AQ2*BQ2+ERHO2)/E2 642
XDIFF=(-AQ1*BQ1-AQ2*BQ2-ERHO2)/E2 643
ERHO3=E1*(AQ1*SIN(ERHO1)-AQ2*COS(ERHO1)) 644
YSUM=(AQ2*BQ1-AQ1*BQ2+ERHO3)/E2 645
YDIFF=(AQ2*BQ1-AQ1*BQ2-ERHO3)/E2 646
ZSUM=ALOG(SQRT(XSUM*XSUM+YSUM*YSUM)) 647
ZDIFF=ALOG(SQRT(XDIFF*XDIFF+YDIFF*YDIFF)) 648
IF(IPICK-2)18,18,16 649
18 RHOS=0.0 650
NQS=0 651
CALL QTEST2(YSUM,XSUM,RHOS,NQS,RADS,LS,MCS) 652
RHOD=0.0 653
NQD=0 654
CALL QTEST2(YDIFF,XDIFF,RHOD,NQD,RADD,LD,MCD) 655
GO TO 20 656
16 RHOS=0.0 657
NQS=0 658
CALL QTEST3(YSUM,XSUM,RHOS,NQS,RADS,LS,CYCLES,IC,JC1S,JC2S, 659
IKCS,J,LCS,MCS) 660
RHOD=0.0 661
NQD=0 662
CALL QTEST3(YDIFF,XDIFF,RHOD,NQD,RADD,LD,CYCLED,IC,JC1D,JC2D, 663
IKCD,J,LCD,MCD) 664
20 SSUM=(AU*ZSUM+AV*RHOS)/A1 665
SDIFF=(AU*ZDIFF+AV*RHOD)/A1 666
TSUM=(AU*RHOS-AV*ZSUM)/A1 667
TDIFF=(AU*RHOD-AV*ZDIFF)/A1 668
D2S=A2*SSUM 669
D2D=A2*SDIFF 670
D2SI=A2*TSUM 671
D2DI=A2*TDIFF 672
IF(ABS(D2SI)-ABS(D2DI))10,10,12 673
10 D2=D2S 674
NQ=NQS 675
D2I=D2SI 676
GO TO 14 677
12 D2=D2D 678
NQ=NQD 679
D2I=D2DI 680
14 GO TO (6,8,8),ISHIFT 681
C 682
C CALCULATING PSI AND DELTA. 683
C 684
8 CP2=EXP(AP2*D2)*COS(BP2*D2) 685
DP2=EXP(AP2*D2)*SIN(BP2*D2) 686
EP2=C3+C7*CP2-C8*DP2 687
FP2=C4+C7*DP2+C8*CP2 688
GP2=1.0+C3*C7*CP2-C3*C8*DP2-C4*C7*DP2-C4*C8*CP2 689
HP2=C3*C7*DP2+C3*C8*CP2+C4*C7*DP2-C4*C8*DP2 690
AKP2=(EP2*GP2+FP2*HP2)/(GP2*GP2+HP2*HP2) 691
ALP2=(FP2*GP2-EP2*HP2)/(GP2*GP2+HP2*HP2) 692
EN2=C1+C5*CP2-C6*DP2 693
FN2=C2+C5*DP2+C6*CP2 694
GN2=1.0+C1*C5*CP2-C1*C6*DP2-C2*C5*DP2-C2*C6*CP2 695
HN2=C1*C5*DP2+C1*C6*CP2+C2*C5*CP2-C2*C6*DP2 696

```

	AKN2=(EN2*GN2+FN2*HN2)/(GN2*GN2+HN2*HN2)	697
	ALN2=(FN2*GN2-EN2*HN2)/(GN2*GN2+HN2*HN2)	698
	RP2=(AKP2*AKN2+ALP2*ALN2)/(AKN2*AKN2+ALN2*ALN2)	699
	SP2=(AKN2*ALP2-AKP2*ALN2)/(AKN2*AKN2+ALN2*ALN2)	700
	ACON=SQRT(RP2*RP2+SP2*SP2)	701
	PSIC=ATAN(ACON)*57.29578	702
	SD=SP2/ACON	703
	CD=RP2/ACON	704
	RHO=0.0	705
	CALL QTEST4(SD,CD,RHO)	706
	DELC=RHO*57.29578	707
6	RETURN	708
	END	709
	SUBROUTINE QTEST(A,B,C)	710
	IF(B)2,4,4	711
2	C=ATAN(A/B)-3.141593	712
	GO TO 6	713
4	C=ATAN(A/B)	714
6	RETURN	715
	END	716
	SUBROUTINE QTEST2(A,B,C,N,RAD,L,MC)	717
	IF(B)2,4,4	718
2	C=ATAN(A/B)-3.141593-RAD	719
	N=2	720
	MC=4	721
	GO TO 6	722
4	C=ATAN(A/B)-RAD	723
	N=3	724
	IF(A)8,10,10	725
8	N=N+1	726
	IF(N-MC)12,14,12	727
6	IF(A)8,12,12	728
10	N=1	729
	JC=N-1+L	730
	IF(JC)14,16,16	731
14	RAD=RAD+6.283186	732
	L=0	733
	MC=0	734
	GO TO 4	735
12	L=-1	736
16	RETURN	737
	END	738
	SUBROUTINE QTEST3(A,B,C,N,RAD,L,CYCLE,IC,JC1,JC2,KC,J,LC,MC)	739
	IF(IC-1)2,2,4	740
2	LC=1	741
4	IF(B)6,8,8	742
6	C=ATAN(A/B)-3.141593-RAD	743
	N=2	744
	GO TO 10	745
8	C=ATAN(A/B)-RAD	746
	N=3	747
	IF(A)12,14,14	748
12	N=N+1	749
	IF(L)16,18,18	750
10	IF(A)12,18,18	751
14	N=1	752
	JC=N-1+L	753
	IF(JC)20,16,18	754

20	RAD=RAD+6.283186	755
	L=1	756
	IF(IC-1)22,22,24	757
22	JC1=2	758
	GO TO 8	759
24	IF(LC)8,8,26	760
26	JC2=2	761
	GO TO 8	762
18	IF(J-1)16,16,28	763
28	L=-1	764
16	IF(IC-KC)30,32,30	765
32	IF(JC2-IC)34,36,36	766
36	IF(N-1)34,34,38	767
38	KC=0	768
	JC2=0	769
	GO TO 40	770
34	C=C+6.283186	771
	CYCLE=CYCLE-6.283186	772
	KC=0	773
	JC1=2	774
	MC=4	775
	GO TO 40	776
30	IF(JC1-IC)40,40,42	777
42	IF(N-1)40,40,44	778
44	C=C-6.283186	779
	CYCLE=CYCLE+6.283186	780
	KC=2	781
	JC1=0	782
40	IF(N-MC)46,48,46	783
48	C=C-6.283186	784
46	IF((IC-1)*LC)50,50,52	785
52	LC=0	786
50	RETURN	787
	END	788
	SUBROUTINE QTEST4(A,B,C)	789
	IF(B)2,4,4	790
4	IF(A)6,8,8	791
8	C=ATAN(A/B)	792
	GO TO 10	793
2	C=ATAN(A/B)+3.141593	794
	GO TO 10	795
6	C=ATAN(A/B)+6.283186	796
10	RETURN	797
	END	798

APPENDIX B. FORTRAN IV Notation

Appendix B presents an explanation of the essential terms used for the source program.

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Note: The index of refraction of a surface film is given by

$$\hat{n}_2 = n_{21} - n_{22}i, \text{ where}$$

n_{21} = real part of the refractive index.

n_{22} = imaginary part of the refractive index.

Variable Name	Explanation	Variable Name	Explanation
ANSETS	Number of values of n_{21} calculated for a set of psi and delta measurements.	EN1	Refractive index of the surrounding medium (n_1).
AVE	Mean value for the final calculation of n_{21} .	EN21	Value of n_{21} . Storage location for the minimum and maximum values of the n_{21} range.
AVE1	Temporary storage location for the beginning mean value calculations of n_{21} .	EN21N	Minimum value of the n_{21} range.
AVE2	Temporary storage location for the maximum value of the n_{21} range.	EN21X	Maximum value of the n_{21} range.
AVEL	Mean value dividing the left side of the reduced n_{21} range.	EN22	Value of n_{22} .
AVEP	Center of the reduced n_{21} range.	EN22N	Minimum value of the n_{22} range.
AVER	Mean value dividing the right side of the reduced n_{21} range.	EN22X	Maximum value of the n_{22} range.
AVN21	Mean value of n_{21} calculated for the set of psi and delta measurements.	EN3	Subroutine subprogram for calculating the refractive index of the substrate, $\hat{n}_3 = n_{31} - n_{32}i$.
CYCLED } CYCLES }	Corrects the cycling of angle phi (subroutine subprogram QTEST3).	EN31	Real part of the refractive index of the substrate (n_{31}).
D2	Real part of film thickness.	EN32	Imaginary part of the refractive index of the substrate (n_{32}).
D2I	Imaginary part of film thickness.	EPSI	Difference between experimental and calculated values of psi ($\delta\psi$).
DEL	Optical parameter, delta (Δ).	ERROR	$\sqrt{(\delta\psi)^2 + (\delta\Delta)^2}$
DELC	Calculated values of delta.	ESUM	$\sqrt{(\delta\psi)^2 + (\delta\Delta)^2}$
DELP	Optical parameter, delta (Δ'), of a "clean" surface.	I	Index variable for controlling the minimum and maximum values of the n_{21} range.
DN21	Increment of n_{21} used to calculate an array of n_{21} values (subroutine subprogram RANGE).	ICOUNT	Number of values of n_{21} calculated for a set of psi and delta measurements.
DN22	Increment of n_{22} used to calculate an array of n_{22} values (subroutine subprogram RANGE).	IDIAG	Code numbers for the resulting n_{21} calculations for psi and delta.
EDEL	Difference between experimental and calculated values of delta ($\delta\Delta$).	IPATH	Variable name for testing for a solution using the minimum and maximum values of the n_{21} range.
		IPICK	Variable name segmenting the main program.
		ISHIFT	Variable name segmenting the subroutine subprogram RID2.

Variable Name	Explanation	Variable Name	Explanation
ITOL	Variable name for the execution of the tolerance level used to determine n_{21} for psi and delta.	MCD } MCS }	Control numbers for determining the quadrant for angle phi (subroutine subprogram QTEST2 and QTEST 3).
IVARI	Control number used to compute and compare error for n_{21} .	MVARI	Control number used to compute and compare error for n_{21} .
J	Index variable for the psi and delta measurements.	N21	Number of n_{21} values computed for a range of n_{21} .
J21	Control number for the n_{21} values in a data set.	N22	Number of n_{22} values computed for a range of n_{22} .
JC1D } JC1S } JC2D } JC2S }	Control numbers for the cycling of angle phi (subroutine subprogram QTEST3).	NQ	Quadrant for the angle phi.
JJ	Control number for the input device.	NSETS	Number of psi and delta measurements.
JVARI	Control number used to compute and compare error for n_{21} .	NTEST	Variable name limiting the cycling for n_{21} .
K	Index variable for values of n_{22} .	NTOL	Control number determining the error for n_{21} .
K22	Control number to determine n_{22} .	NUMBER	Number of data sets to be processed.
KCD } KCS }	Control numbers for the cycling of angle phi (subroutine subprogram QTEST3).	OPN21	Value of n_{21} determined for a psi and delta measurement. Value of n_{21} .
KK	Control number for the output device.	PHI1	Angle of incidence (ϕ_1).
KVARI	Control number used to compute and compare error for n_{21} .	PSI	Optical parameter, psi (ψ).
L	Index variable for the error term ϵ . Index variable for the final calculation of n_{21} .	PSIC	Calculated values of psi.
LABEL	Data set identification.	PSIP	Optical parameter, psi (ψ'), of a "clean" surface.
LCD } LCS }	Control numbers for the cycling of angle phi (subroutine subprogram QTEST3).	QTEST	Subroutine subprogram for correcting the quadrant of angle phi.
LD } LS }	Control numbers for determining the quadrant for angle phi (subroutine subprogram QTEST2 and QTEST3).	QTEST2	Subroutine subprogram for correcting the quadrant of angle phi and controlling the cycling of angle phi.
LVARI	Control number used to compute and compare error for n_{21} .	QTEST3	Subroutine subprogram for correcting the quadrant of angle phi, controlling the cycling of angle phi and maintaining the simultaneous theoretical cycling of the angle phi for minimum and maximum values of n_{21} , for each psi and delta measurement.

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Variable Name	Explanation	Variable Name	Explanation
QTEST4	Subroutine subprogram for selecting the quadrant for the optical parameter, delta (Δ).	SIGMA	Standard error for the mean n_{21} value calculated for a set of psi and delta measurements.
RADD } RADS }	Control numbers for the cycling of angle phi (subroutine subprogram QTEST2 and QTEST3).	SUM1 } SUM2 }	Variable names used to compute standard error.
RANGE	Subroutine subprogram for calculating the number of n_{22} values and the number of n_{21} values from their respective ranges.	TOL	Tolerance level given to determine n_{21} .
RID2	Subroutine subprogram for calculating film thicknesses and the psi (ψ) and delta (Δ) optical parameters.	WAVE	Wavelength (λ) of the light beam.