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A FORTRAN PROGRAM FOR ANALYSIS OF ELLIPSOMETER MEASUREMENTS AND CALCULATION OF REFLECTION COEFFICIENTS FROM THIN FILMS

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U. S. DEPARTMENT OF COMMERCE NATIONAL BUREAU OF STANDARDS

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# NATIONAL BUREAU OF STANDARDS Technical Note 242

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Frank L. McCrackin

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#### A Fortran Program for Analysis of Ellipsometer Measurements and Calculation of Reflection Coefficients from Thin Films

Frank L. McCrackin

A Fortran computer program to calculate the reflection coefficients for both single and multiple thin films and to analyze optical measurements of such films by an ellipsometer is presented. Both the films and the substrate may be absorbing and have complex indexes of refraction. The reflection coefficients of inhomogeneous films (films of varying refractive index) may be computed by determining the reflection coefficients of an equivalent series of homogeneous films.

The ellipsometer measurements for a given film may be calculated or the index of refraction and thickness of a film may be calculated from ellipsometer readings. The ellipsometer measurements may be corrected for the retardation of the compensator or for multiple reflections of the light.

#### 1. Introduction

The reflection of light from surfaces and thin films has been discussed by various authors [1,2]. The reflection is expressed in terms of the reflection coefficients R<sup>p</sup> for light polarized parallel to the plane of incidence and R<sup>S</sup> for light polarized perpendicular to the plane of incidence. Since these coefficients are complex quantities, they represent both the change of amplitude and phase of the light on reflection.

The ellipsometer is an optical instrument used to study surfaces and their films by reflection of light [3,4]. The ellipsometer measures the ratio of the reflection coefficients

$$\rho = \frac{R^{p}}{R^{s}} = \tan \psi e^{i\Delta}$$

The ellipsometer contains a polarizer, analyzer, and compensator. For the commonly occurring case of the relative retardation Q of the compensator equal to 90°, and the arrangement of components given by reference 3,  $\rho$  is related to the settings of the polarizer P and the analyzer A by

$$P = \Delta/2 - 45$$

The ratio of reflection coefficients, p, is a function of the refractive index of the substrate,  $n_3$ , (which may be complex) the thickness  $d_j$ , and refractive index  $n_j$  of any of <u>j</u> films on the surface, some or all of which may be complex, the refractive index of the surrounding medium,  $n_1$ , the angle of incidence,  $\varpi_1$ , the wavelength of the light used, and the retardation of the quarter wave plate. Hence the ellipsometer readings P and A are related to the optical constants of a surface and the thickness and index of refraction of films on the surface. However, since the calculations required to determine these quantities from ellipsometer measurements (and also the inverse calculations) are very time consuming, this Fortran program was consequently developed for this purpose.

The following computations can be performed by this program:

1) Computation of ellipsometer readings and reflection coefficients for given refractive indexes of surrounding medium, film and substrate and given film thickness.

2) Computation of film thickness from ellipsometer readings for given refractive indexes of film and substrate

3) Computation of film thickness and refractive index of film from ellipsometer readings for given refractive index of substrate.

4) Computation of refractive index of a bare substrate from ellipsometer readings.

## 2. Methods of Calculation

Most of the formulas used in this program are given in McCrackin et al [3]. The correction of ellipsometer readings for a compensator which has a retardation other than quarter wave, is given by Winterbottom [2]. The calculations involved in use of multiple reflections of the light from several surfaces as well as discussion of increase of sensitivity and experimental technique is given by Stromberg et al [5]. The calculation from P and A of the thickness of a film of given refractive index (Instructions No. 903) has also been described by McCrackin et al [3].

I will now describe briefly the manner of introducing data and instructions into the computer and some of the calculations which may be performed by this program; a

detailed discussion of the program will be found in the Section entitled "Computer Instructions".

The first card for any calculation is a title card that contains any desired identifying information. Following cards start with an instruction number in columns 1 to 3 of the cards, followed by numbers starting in columns 10, 20, 30, 40, 50, and 50. All numbers except the instruction number must contain a decimal point. The instruction number determines the meaning of subsequent numbers and the calculation (if any) to be performed. Instruction numbers from 001 to 901 are used to introduce data; those from 902 to 907 instruct the computer to perform a certain calculation.

For a substrate without a film, the ratio of reflection coefficients,  $\rho$ , depends on the angle of incidence,  $\phi$ , of the light, the refractive index,  $n_1$ , of the surrounding medium, and the refractive index,  $n_3$ , of the substrate. The refractive index of the substrate,  $n_3$ , may be calculated from the reasured value of  $\rho$  (given by values of P and A),  $\phi$  and  $n_1$ . This calculation is done by the instruction number 905 after  $\phi$  and  $n_1$  have been given by a OOl instruction.

For a film on a substrate, ellipsometer readings P and A and the reflection coefficients may be computed from  $\phi$ ,  $n_1$ ,  $n_3$ , and the thickness,  $d_2$ , and refractive index,  $n_2$ , of the film. This calculation is performed by the 902 instruction after  $n_1$  and  $\phi$  are given by an OOl instruction,  $n_2$  is given by an OO2 instruction, and  $n_3$  is given by an OO3 instruction. The thickness  $d_2$  is given by the 902 instruction. Alternatively, the thickness of a film,  $d_2$ , may be computed from P, A,  $\phi$ ,  $n_1$ ,  $n_2$ , and  $n_3$  by instruction after  $\phi$  and  $n_1$  are given by an OOl instruction,  $n_2$  is given by an 0.02 instruction, and  $n_3$  by instruction after  $\phi$  and  $n_1$  are given by an OOl instruction.

For a non-absorbing film, with real index of refraction, both  $d_2$  and  $n_2$  may be computed by the 90<sup>4</sup> instruction. The P and A values are given by the 90<sup>4</sup> instruction after  $\phi$  and  $n_1$  are given by an OOl instruction,  $n_3$  by an OO3 instruction, and a range of values that includes the solution for  $n_2$  by the OO2 instruction.

The required instructions to perform some typical calculations for single films are now described. The Section entitled "Computer Instructions" gives detailed instructions for the similar calculations for multiple films as well as the other calculations that may be performed by this program.

2.1 Calculation of Ellipsometry Readings and Reflection

Coefficients for a Film Covered Surface

Instruction number 902 will cause the computer to calculate the ellipsometer readings and reflection coefficients for reflection of light from a film-covered surface. The thickness of the film is given with the 902 instruction card. Before the 902 instruction, instructions 001, 002, and 003 must be used to give the other values required for the calculation. The OOl instruction gives the index of refraction of the medium above the film, the angle of incidence of the light, and the wavelength of the light. The 002 instruction gives the index of refraction of the film and the 003 instruction gives the index of refraction of the substrate. Also, every calculation must be terminated by a 910 instruction. For example, let light of wavelength 4800 A be incident at 65° in air on a film covered surface. Let the thickness of the film be 40 A, the refractive index of the film be 1.4, and the complex refractive index of the substrate be 3.316-4.383 i. The following input data computes the ellipsometer reading, P and A, and the reflection coefficients,  $R^p$  and  $R^s$ :

	Column No.			
1	10 2	20	30	
JONES	TEST CALCULATION			3-10-64
001	l.	65.	4800.	
002	1.4	<b>D D C</b>	1	
003	(blank)	3.316	4.333	
902	40.			
910				

Notice that the absolute value of the imaginary component of the refractive index is used.

Tables of ellipsometer readings and reflection coefficients for films of different thicknesses and refractive indexes may also be computed by the 902 instruction. In this case, the initial value, increment, and final value to be used are given for the thickness and refractive index of the film. Thus, the input data:

1	Column No. 10	20	30	
JONES 001 002 003 902 910	TEST CALCULAT: 1. 1.4 (blank) 0.	ION 65. 0.1 3.316 20.	4800. 1.6 4.383 100.	3-10-64

will produce tables for films of refractive index of 1.4, 1.5, and 1.6 for each table, the ellipsometer readings and reflection coefficients will be given for films 0., 20., 40., 60., 80., and 100 Å thick.

Calculations may also be performed for absorbing films of complex refractive index, as described in the section entitled, "Computer Instructions".

# 2.2 Calculation of Index of Refraction for Film-Free

Substrate from Ellipsometer Readings

Instruction 905 calculates the index of refraction of a film-free surface from ellipsometer readings P and A. The index is printed and may also be used in the following calculations.

2.3 Calculation of Film Thickness from Ellipsometer Readings for Given Index of Refraction of Film

Instruction 903 computes the thickness of a film from ellipsometer readings P and A. The OOl and OO2 instruction must precede this instruction and the index of the substrate must have been either given by a OO3 instruction or calculated by a 905 instruction. For example, suppose a filmfree surface was measured under water (refractive index of 1.33) to give P = 27.32° and A = 30.45°. Then an absorbing film of refractive index 2.5 - 0.3 i was placed on the surface and reading of P = 31.15 and A = 29.00° were obtained. Let the angle of incidence be 65° and the wavelength of the light be 4800 Å in vacuum. The following input data will calculate the thickness of the film: Column No.

1		10		20	30	40
001 905 002 903 910	JONES	CAL 1, 27 2, 31	FILM 33 7.32 5 1.15	THICKNESS 65, 30.45 (blank) 29.00	4800. (blank)	.3

If the 002 instruction specifies a series of values for the refractive index of the film, a film thickness can be computed using each value of the series for the refractive index of the film.

These examples illustrate the manner in which the input data is written. Instructions are also available to do calculations for multiple films, to calculate the index of refraction of adsorbed films, to determine ranges of error of the calculated refractive index of a film, to correct the ellipsometer readings for reflection of light from multiple surfaces, and to correct the ellipsometer readings for a compensator of arbitrary relative retardation. A detailed explanation of all the instruction numbers, a list of subroutines used by the program, a list of variables used in the program, the fortran program, and a flow diagram of the program follow.

#### 3. Computer Instructions

This program can perform calculations for reflection of light from one to 898 films. The case of five films is shown in Figure 1.

The refractive indices are labelled  $n_1$  to  $n_7$  and the thicknesses of the films are  $d_2$  to  $d_6$ . The index  $n_1$  of the medium is assumed real, but all the other indices may be complex. The angle of incidence of the light in the medium is  $\phi$ , and is measured in degrees. The vacuum wavelength of

the light is  $\lambda$ . The film thicknesses and  $\lambda$  must be expressed in the same units. The relative retardation of the quarter wave plate in the ellipsometer is Q, measured in degrees, and is assumed to be 90° unless otherwise specified.

The first line of the data is a title identifying the run. Each following line (or card) of data consists of an instruction number followed by the data. Each instruction number determines the meaning of subsequent data and the calculation to be performed. The instructions are as follows:

Instruction No. 001

This instruction gives values of  $n_1$ ,  $\phi$ ,  $\lambda$ ,  $\alpha$ , number of reflections, and Q for use in later calculations.  $n_1$  is the refractive index of the surrounding medium,  $\dot{\phi}$  is the angle of incidence,  $\lambda$  is the wave length of the light in vacuum,  $\alpha$  is a number used to control the calculations for instruction No. 904 and will be discussed under instruction.904, and Q is the relative retardation of the compensator used in the ellipsometer. The instruction reads as follows:

	Column No.						
1	10	20	30	40	50		60
001	nl	¢	λ	α	No ref	lections	ر م

The computer assumes the initial values

- $n_1 = 1$
- $\phi = 70^{\circ}$
- $\lambda = 5461.$

 $\alpha = 0$ 

No. of Reflections = 1

and if these values are to be used, the instruction OOl does not need to be given. Also, values need be given only when they are to be changed. Thus, to give the values  $n_1 = 1.5$ ,  $\phi = 65^\circ$ ,  $\lambda = 5461$ ,  $\alpha = 0$ , number of reflections = 5, and  $Q = 90^\circ$ , the instruction would be

CO]	umns
-----	------

1	10	20	30	40	50	60
001	1.5	65.			5.	

If later calculations were to be performed for the same values except that  $\phi$  is changed to 75°, the required 001 instruction is

Columns

10 20

001 75.

Notice that, except for instruction numbers, all numbers given as input data must have a decimal point.

#### Instruction No. 002

This instruction gives values of the index of refraction,  $n_2$ , of the top film for use in following calculations. If only real values of  $n_2$  are to be used, the arrangement of the 002 card is

Columns 1	10	20		30		
002	Initial	Increme	ent	Final		
	n <sub>2</sub>			<sup>n</sup> 2		
For	example,	to specify	<sup>n</sup> 2 =	3, 3.5	and 4,	the
instruct:	ion is:					
Columns 1	10	20	30			
002	3.	•5	4.			

To specify complex values of the refractive index, the values to be used for the imaginary component are specified after the real component. For example, the card:

С	0]	un	n	ន
-				

1	10	20	30	40	50	60
002	3.	•5	4.	0.	.1	.2

will cause all following calculations to be done for these values of n<sub>2</sub>:

3.	3.5	4
3-0.1 i	3.5-0.1 i	40.1 i
3-0.2 i	3.5-0.2 i	4 -0.2 i

A single value for the refractive index may be given by omitting the increment and final value for the real and imaginary component. Thus the value  $n_2 = 3-i$  is specified by:

Columns							
1	10	20	30	40	50	60	
002	3.			1.			

#### Instructions No. 003 to 900

These instructions give the thicknesses and indices of the films and substrate. Thus, if film number 4 was 100 Å thick with an index of 1.4 - 2.2 i, the line of data would be

004 100. 1.4 2.2

No thickness is given for the substrate. An instruction for a film may be repeated. For example, for five films with medium and substrate lines with instruction numbers 001 to 007 would be given. These would be followed by instructions causing calculations. Then the thickness and index of any film could be changed by repeating its instruction number and additional calculations could be performed with the original values for the other films. For more than one film, the last of these cards must contain 1. starting in column 40 on the card.

Instruction No. 901

This instruction gives values of  $\rho_1$ ,  $\rho_p$ ,  $n_p$ ,  $\delta$  P, and  $\delta$ 'A to be used in subsequent calculations. The values  $\rho_1$ ,  $\rho_p$  and  $n_p$  are used to compute the mass of material per unit area of the film for instructions 903 and 904. The values  $\delta$ 'P and  $\delta$ 'A are used by instruction 904. If this instruction is used, all values must be given.

#### Instruction No. 902

This instruction causes the computer to calculate tables of P, A, and reflection coefficients for the films. The

range of thicknesses of the upper film are given on the line. Thus

902 0. 5. 15.

will cause the calculation for  $d_2 = 0., 5., 10$ , and  $15 \Lambda$ and for all values of  $n_2$  given previously.

The values of d<sub>2</sub> may be omitted from the 902 instruction if they have been previously given. For example, a section of data may be

001 1.3

902 0, 10. 100.

001 1.4

902

001 1.5

902 100. 10. 200.

910

Tables of P and A will be printed for  $d_2 = 0$  to 100 in steps of 10 for  $n_1 = 1.3$  and 1.4, and for d = 100 to 200 in steps of 10 for  $n_1 = 1.5$ . Instruction No. 903

In this case, readings P and A are given. The computer calculates and prints a value of  $d_2$  to give the best fit [3] to the P and A readings for every  $n_2$  given by the OO2 instruction. It also computes the value of P and A corresponding exactly to the  $n_2$  and  $d_2$  values and prints the differences  $\delta P$  and  $\delta A$  between these computed P and A

values and the P and A readings.

Two solutions for  $d_2$  and a measure of error for each solution are computed by the method given in reference 3. These solutions are obtained as solutions of a quadratic equation by taking the plus or minus sign for the radical. The solution with the smallest measure of error, labeled THICK, with its measure of error, labeled ERROR, and  $\delta P$  and  $\delta A$ , labeled DEL P and DEL A, are printed on the left hand side of the printout, and the sign of the radical for this solution is printed to the extreme right of the printout. The other solution for the thickness with corresponding values of  $\delta P$ ,  $\delta A$  and measure of error are printed on the right hand side of the printout.

If the film is not compact but is a mixture of the surrounding medium and a material of density  $\rho_p$  and refractive index  $n_p$ , the mass of material per unit area of the film is computed in mg/cm<sup>2</sup> and is printed. The value of  $\rho_1$ , density of surrounding medium g/cm<sup>3</sup>,  $\rho_p$  in g/cm<sup>3</sup> and  $n_p$  are given by the 901 instruction; the Lorentz-Lorentz equation is used to compute the refractive index of the film.

If compensator with retardation other than  $90^{\circ}$  is used, values of P, a and a must be given (listed in this order) instead of merely P and A [2, 3].

Instruction No. 904

The measured values of P and A are given. The computer determines the film index,  $n_2$ , and film thickness corresponding to the values of P and A, if a solution for  $n_2$  exists in the range of values given for  $n_2$  by the previous 002 instruction. If  $n_2 = n_{2r}$ - in<sub>2i</sub> is complex and a range of values of  $n_{2i}$  has been specified by a 002 instruction, a value of  $n_{2r}$  will be computed for each of the values of  $n_{2i}$  specified.

The computer finds the solution for nor by computing the film thickness for assumed values of  $n_{2r}$  [3]. This computed thickness is a complex number. The real part of the computed thickness is chosen as the film thickness and the imaginary part,  $d_i$ , as a measure of error. Then the P and A values are calculated for this film index and real thickness and their differences  $\delta P$ ,  $\delta A$  from the given values of P and A are computed. These differences are then compared with the allowed differences  $\delta$  P and  $\delta$  A given by the 901 instruction. If the differences  $\delta P$  and  $\delta A$  are both smaller (in absolute value) than the allowed differences  $\delta'P$  and  $\delta'A$ , the computer prints the results of the calculation for this value of nor; otherwise a new value of  $n_{\mbox{2r}}$  is chosen and the calculation repeated until  $\delta P$  and  $\delta A$ are smaller than  $\delta$  P and  $\delta$  A.

If values of  $\delta' P$  and  $\delta' A$  have not been given by a 901 instruction, the computer assumes  $\delta' P = \delta' A = .0005^{\circ}$ .

In particular, the film thickness and error terms  $\delta P$ ,  $\delta A$  and  $d_{1}$  are first computed for the initial and final values of nor given by the previous 002 instruction. The two error terms d, for the two values of n2r are examined. Since d, must be zero for the correct value of nor, it is expected to change sign as nor varies from the initial to final value of the specified range. Therefore, if the d, values for the initial and final values of nor have the same sign, the computer assumes that there is no solution within the specified range of nor. The information printed for this case is determined by the sign of  $\alpha$  as given by a previous OOl instruction. If it is not specified or  $\alpha$  is positive, no printout is given. However, if a has a negative value, the comment "No solution in range of no" is printed and the results of the calculation for the initial and final values of nor are printed. If the range of values for nor specified by the 002 instruction is too large, two or more solutions for n<sub>2r</sub> may occur in the range of n2r, so the error term d, may have the same sign at each end of the range of nor. In this case, the computer will erroneously assume that there is no solution in the range of normal is only occurred when no is complex.

However, if d, has different signs for the initial and final values of nor, the computer performs the calculations for a value of nor equal to the average of the two previous values of  $n_{2r}$ . If the error terms  $\delta P$  and  $\delta \Lambda$  for this solution are less than  $\delta$ 'P and  $\delta$ 'A, the computer prints the solution. Otherwise, it determines in which half of the range of no the solution lies. If the signs of d, for initial, average, and final values of the refractive index of the film are + -- or -++, the solution for n2 lies between the initial and average values, otherwise the solution lies between the average and final values. Using this reduced range for no the procedure is repeated until the error terms  $\delta P$  and  $\delta A$  are less than  $\delta P$  and  $\delta A$  in absolute value. The procedure will be repeated only 20 times as a precautionary measure against use of excessive computation time.

Thus an index of refraction  $n_2$  and thickness of a film is computed from measured values of P and A. This value of  $n_2$  is the best value determined from the measured P and A values but will contain an error due to errors of measurement of the P and A values. The computer will determine the limits of error for  $n_{2r}$  from the limits of error of P and A if a value for  $\alpha$  has been previously given. The upper limit of error is determined first. The increment of  $n_{2r}$  (given by preceding 002 instruction) is added to the

best value of  $n_2$  and film thickness and error terms computed for this value. If the error term in either P ( $\delta$ P) or A( $\delta$ A) is larger than the limit of experimental error of P and A, this value of  $n_{2r}$  is taken as the upper limit for  $n_{2r}$ . Otherwise, the increment of  $n_{2r}$  is again added and the process repeated. This process is repeated until one of three things occur:

(1) Either error term is larger than the experimental error of P or A.

(2) The value of  $n_{2r}$  is larger than the upper limit for  $n_{2r}$  (given by 002 instruction).

(3) The process has been performed  $\alpha$  times. (The absolute value of  $\alpha$  is taken, as  $\alpha$  may be negative).

The value of  $\alpha$  is, of course, given by the OOl instruction. A value of 20 for  $\alpha$  has been found to be satisfactory.

The lower limit for  $n_2$  is determined similarly with the increment of  $n_2$  subtracted instead of added. In this case, the calculation stops if the value of  $n_2$  is less than the lower limit for  $n_2$ .

If a compensator with a retardation different from  $90^{\circ}$  is used in the ellipsometer, values of p,  $a_{p}$ , and  $a_{s}$  (listed in this order) instead of P and A must be given with this instruction.

Instruction No. 905

This instruction calculates the index of the substrate from P and A readings of the bare substrate. The index of the substrate may be given by an instruction 003 to 900 or computed by this instruction. If the retardation of the compensator is different than 90°, values of p, a<sub>p</sub>, and a<sub>s</sub> must be given.

#### Instruction No. 906

The experimental errors of P and A are given. These are used for instruction 904 when  $\alpha$  has been given. Instruction No. 907

Experimental values of p,  $a_p$ , and  $a_s$  are given and the value Q of the compensator is calculated. The notation and equations are given by Winterbottom [2]. Instruction No. 908

This instruction allows another title card to follow it. Instruction No. 909

This instruction sets all the values that have been given by instructions 001, 902, and 906 to their initial values. It is followed by a title card.

The number of films may be increased by giving instructions 003 to 900, but may not be decreased. Suppose, for example, the system of 5 films previously shown (with refractive indexes  $n_2$  to  $n_7$ ) has been given to the computer. Then to describe a system of 7 films (indexes  $n_1$  to  $n_9$ )

instructions 003 and 009 with instructions for any other films that are to be changed in thickness of index are all that are required. However, to describe a system of less than 5 films, instruction 909 must be used. Instruction No. 910

This instruction stops the calculation. It must be the last instruction of every set of data.

To perform calculations involving multiple reflection of the light, or where an imperfect quarter wave plate  $(Q \neq 90^{\circ})$  has been used, the number of reflections or value of Q are given by OOl instruction. For an imperfect quarter wave plate, values of P,  $a_p$ , and  $a_s$  are given with instructions 903, 904, and 905, also the value of Q may also be computed by a 907 instruction.

Every set of data must start with a title card and instructions 908 and 909 must be followed by a title card. A title card may contain any information desired in columns 1 to 80.

The program is written in Fortran II for use on IBM machines 704, 7090 or 7094 with the Bell Monitor. For use with other Monitors, the READ, PRINT, and CALL SYSTEM statements would have to be changed.

4. Functions and Subroutines for Ellipsometry Program ABSF Absolute value SORTE Square root Sine of argument in radians SINF Cosine of argument in radians COSF SINDF Sine of argument in degrees COSDF Cosine of argument in degrees LOGF Logarithm to base e Arctangent, result in degrees ATANDF  $ATN_{F}(Y,X)$ Arctangent of Y/X with result in proper quadrant in radians SYSTEM End of computation Complex square root, square root of a CSR complex no. CD Complex division Complex multiplication CM CS(C3, X, FN3)Cosine of angle of propagation of light

$$C3 = \sqrt{1 - (n_1 \sin \phi_1/n_3)^2}$$

 $X = n_1 \sin \phi_1, FN3 = n_3; n_3 \text{ and } C \text{ 3 complex numbers}$ SRC(R, T1, T2) Small reflection coefficient R, T1, T2 complex  $R = \frac{T1 - T2}{T1 + T2}$ 

I.C(CR, RP21, RP32, Q) Capital reflection coefficient  
CR, RP21, RP32, and Q are complex  

$$P = 4\pi Q$$
  
 $CR = \frac{RP21 + RP32 e^{-iP}}{1 + RP21 * RP32 e^{-iP}}$   
 $Q = \frac{n_2 \cos \phi_2 d_2}{\lambda}$ 

5. Variables Used in Fortran Program

Dimensional Variables

B(2)	Coefficient in equation for y
C(2)	Coefficient in equation for y
C2(2)	Cos $\phi_2$
C3(3)	Cos \$3
CI(2)	Cos $\phi_i$
CIPJ(2)	Cos $\phi_{n+1}$
CM(2)	Cos $\phi_n$
CNM1(2)	Cos $\phi_{n-1}$
CRN(2)	Total reflection coefficient (normal
CRN21(2)	Total reflection coefficient between films 2 and 1 (normal polarization)
CRN32(2)	Total reflection coefficient between films 3 and 2 (normal polarization)
CRP(2)	Total reflection coefficient (parallel
CRP21(2)	Total reflection coefficient between films 2
CRP32(2)	Total reflection coefficient between films 3
D(900)	and 2 (parallel polarization) d <sub>L</sub> thickness of film L
D2C(2)	d <sub>2</sub> computed from y <sub>1</sub>
D20X(2)	d <sub>2</sub> computed from y <sub>2</sub>

DF,N5(5)	Increment for film refractive index
E(2)	Coefficient in equation for y
FN2(2)	n2 refractive index of upper film
FN2E(2)	Final value for film refractive index
FN2I(2)	Initial value for film refractive index
FN2X(2)	n <sub>2</sub> with imaginary part positive
FNX(900,2)	$n_L^{-}$ refractive indexes of film $_L$
IDT(12)	Title
RHO <b>(2)</b>	$\rho = \frac{R^{p}_{21}}{R^{n}_{21}} = \tan \psi e^{i\Delta}$
RN <b>(2)</b>	r <sup>n</sup> n-l,n reflection coefficient between sub- strate and adjacent film (normal polarization)
RN21(2)	r <sup>n</sup> 21 reflection coefficient between films 2 and 1 (normal polarization
RN32(2)	$r_{32}^n$ reflection coefficient between films 3 and 2 (normal polarization)
RP(2)	r <sup>p</sup> n-l,n reflection coefficient between sub- strate and adjacent film (parallel polarization)
RP21(2)	r <sup>p</sup> <sub>21</sub> reflection coefficient between films 2 and 1 (parallel polarization)
RP32(2)	r <sup>p</sup> <sub>32</sub> reflection coefficient between films 3 and 2 (parallel polarization)
T1(2) to T5(2)	Temporary storage for complex numbers
XX(5)	Ln(-y)
A5(5) A1(5)	Solutions for $y = e^{-4\pi i n 2} \cos \phi_2 d_2 / \lambda$ of equation Ey <sup>2</sup> + By + C = 0

# NON-DIMENSIONAL VARIABLES

A	А	Angle of analyzer
ADX	Acal <sup>-A</sup> exp	Difference between calculated and experimental values of A
AP	Ap	
AS	As	
ХA		Calculated A for single and multiple reflections
AXX	Measured A	
СІ	$\cos \phi_1$	
DC	А	Adsorption of polymer
DD2	Increment of $d_2$	
DEL	= 2P + 90°	Relative phase retardation
DENP	٩p	Density of polymer
DENI	٩٦	Density of solvent
Dl	d <sub>2</sub>	Computed film thickness
D2	d <sub>2</sub>	Thickness of upper film
D2F	Final d <sub>2</sub>	
DSI	Initial d <sub>2</sub>	
EA EP		Experimental errors in A and P, used for calculating allowed range of values for film thickness
ERA ERP	$\triangle A$ $\triangle P$	Allowed errors in A and P for cal- culating n <sub>2</sub>
ER1 ER2 ER3		Errors in $d_2$ for real part of $n_2 = X_1, X_2, \text{ and } X_3$
FN		Number of reflections
FNP	np	Index of polymer

FN1	nl	Refractive index of surrounding mediu
HOLD		Temporary storage
I		Index and n-2
J		Index
L		Instruction numbers
M	L-900	Reduced instruction numbers
MIX		Index for computed go to
MY		Index for computed go to
N		Number of layers
NX	N-4	
P	P	Angle of polarizer
PDX	Pcal <sup>-P</sup> exp	Difference between calculated and experimental values of p
PX	Р .	Calculated p for single and multiple reflections
PXX	P	Corrected for quarter wave plate
PHII	0 <sub>1</sub>	Angle of incidence
QWP	Q or $\delta K$	Retardation of compensator
Sl	Sin $\phi_1$	
THETAL	θ	Phase of R <sup>p</sup> 21
Theta2	θ2	Phase of R <sup>n</sup> 21
TNA	Tan A	
TNPSI	Tan ↓	
ЫГ	λ	Vacuum wavelength of light
WP		Used in computing DC
Х	n <sub>l</sub> Sin¢ <sub>l</sub>	
XMl		Magnitude of R <sup>p</sup> 21

XM2		Magnitude of R <sup>n</sup> 21
X1 X2 X3		Trial values of real part of n <sub>2</sub>
XXL	1	Winterbottom
Z	+ or -	Sign used in solution of quadratic eq.
Zl to	Z6	Temporary storage for input data

6. FORTRAN PROGRAM

```
DIMENSION CRN(2), CN(2), RN(2), RP(2), FNX(2,900), D(900), XX(2)
    DIMENSION FN2(2), FN2I(2), DFN2(2), EN2E(2), FN2X(2), C2(2), C3(2)
    DIMENSION RP21(2), RN21(2), RP32(2), RN32(2), Y1(2), Y2(2), E(2), B(2)
    DIMENSION C(2), T1(2), T2(2), T3(2), T4(2), T5(2), RHU(2), IDT(14), CRP(2)
    DIMENSION D2C(2), D2CX(2), CRN32(2), CRP32(2), CRN21(2), CRP21(2)
    DIMENSION Q(2), CNM1(2), CI(2), CIP1(2)
 10 FN1=1.
    PHI1=70.
    WI = 5461.
    DEN1=1.
    DENP=1.
    FNP=1.5
    N = 3
    ERP=.0005
    ERA=.0005
    D2I=0.
    DD2=0.
    D2F=0.
    NCH=0.
    QWP=0.
    FN=1.
    EP=.006
    EA=.02
 20 READ 30, IDT
 30 FORMAT(13A6, A2)
    PRINT 40, IDT
 40 FORMAT(1H113A6, A2, 38H PROG. 10 MULTIPLE FILM ELLIPSOMETRY)
 50 READ 60.L., Z1, Z2, Z3, Z4, Z5, Z6, Z7, Z8
 60 FORMAT(I3,6X,6F10.0,A6,A5)
    PRINT 70, L, Z1, Z2, Z3, Z4, Z5, Z6, Z7, Z8
 70 FORMAT(1H0I3,6F12.5,3X,A6,A5)
    IF(L-1)80,170,80
 80 IF(L-2)90.290,90
 90 IF(L-90)120.120,100
100 M=1-900
    IF(M-9)101,101,550
101 GO TO(110,1050,1100,1100,1100,2070,670,20,10),M
110 DEN1= Z1
    DENP = Z2
    FNP = Z3
    ERP= Z4
    ERA = Z5
    GO TO 50
120 D(L) = Z1
    FNX(1,L) = Z2
    FNX(2,L) = -ABSF(Z2)
    N= XMAXOF(N,L)
    IF(Z4)130,50,130
130 X= S1*FN1
    CALL CS(CN,X,FNX(1,N))
    CALL CS(CNM1+X,FNX(1+N-1))
    CALL CM(T1,FNX(1,N),CNM1)
    CALL CM(T2,FNX(1,N-1),CN)
```

```
CALL SRC(CRP,T1,T2)
    CALL CM(T1,FNX(1,N-1),CNM1)
    CALL CM(T2,FNX(1,N),CN)
    CALL SRC(CRN,T1,T2)
    IF(N-4)160,160,140
140 NX = N - 4
    I = N - 2
    DO 150 J=1,NX
    CALL CS(CIP1, X, FNX(1, I+1))
    CALL CS(CI,X,FNX(1,I))
    CALL CM(T1,FNX(1,I+1),CI)
    CALL CM(T2,FNX(1,I),CIP1)
    CALL SRC(RP,T1,T2)
    CALL CM(T1,FNX(1,I),CI)
    CALL CM(T2,FNX(1,I+1),CIP1)
    CALL SRC(RN,T1,T2)
    Q(1)=T2(1)*D(I+1)/WL
    Q(2)=T2(2)*D(I+1)/WL
    CALL RC(CRN, RN, CRN, Q)
    CALL RC(CRP,RP,CRP,Q)
150 I = I - 1
160 GO TO 50
170 IF(Z1)180,190,180
180 FN1=Z1
190 IF(Z2)200,210,200
200 PHI1= Z2
210 IF(Z3)220,230,220
220 WL= Z3
230 IF(Z4)240,250,240
240 NCH=Z4
250 \text{ S1} = \text{SINDF}(\text{PHI1})
    C1= COSDF(PHI1)
    IF(Z5)260,270,260
260 FN= Z5
270 IF(Z6) 280,275,280
275 QWP=Z6
280 IF(N-4) 50,130,130
290 \text{ FN2I}(1) = \text{ABSF}(21)
    DFN2(1) = Z2
    FN2E(1) = Z3+DFN2(1)/2.
    FN2I(2) = ABSF(Z4)
    DFN2(2) = Z5
    FN2E(2) = Z6+DFN2(2)/2.
    GO TO 50
320 IF(Z1)321,322,321
321 D2I= Z1
322 IF(Z2)323,324,323
323 DD2= Z2
324 IF(Z3)325,400,325
325 D2F= Z3+DD2/2.
    GO TO 400
380 I=N-2
    PRINT 390, I, FNX(1,N), FNX(2,N), FN, P,A
390 FORMAT(1H0I3,23H FILMS, INDEX SUBSTRATE=2F9.5,2H I,F5.0,13H REFLECT
   1IONS.2X,2HP=F9.3,2X,2HA=F9.3/9HO THICK3X,9HA MG/CMSQ4X,5HDEL P4X
```

```
2,5HDEL A6X,5HERROR4X,5HTHICK4X,5HDEL P4X,5HDEL A6X,5HERROR3X,16HN2
   3 REAL N2 IMAG)
400 \text{ EN2X(1)} = \text{EN2I(1)}
    FN2X(2) = FN2I(2)
410 \text{ FN2(1)} = \text{FN2X(1)}
    FN2(2) = -FN2X(2)
    1.1X = -1
420 X= FN1*S1
    CALL CS(C2,X,FN2)
    CALL (S(C3, X, ENX(1, 3)))
    T1(1) = FN2(1) * C1
    F1(2) = FN2(2)*C1
430 T_2(1) = FN1 * C_2(1)
    T_2(2) = FN1 * C_2(2)
    CALL SRC(RP21,T1,T2)
    CALL CM(T2,FN2,C2)
    T1(1) = FN1*CJ
    T1(2) = 0.
    CALL SRC(RN21,T1,T2)
    IF(N-3)550,440,450
440 CALL CM(T1, FNX(1,3), C2)
    CALL CM(T2, EN2, C3)
    CALL SRC(CRP32,T1,T2)
    CALL CM(T1,FN2,C2)
    CALL CM(T2,FNX(1,3),C3)
    CALL SRC(CRN32,T1,T2)
    GO TO 470
450 CALL CM(T1, FNX(1,3), C2)
    CALL CM(T2, EN2, C3)
    CALL SRC(RP32,T1,T2)
    CALL CM(T1, EN2, C2)
    CALL CM(T2, FNX(1,3), C3)
460 CALL SRC(RN32, T1, T2)
    CALL CM(T1,FNX(1,3),C3)
    T_2(1) = T_1(1) * D(3) / WL
    T_2(2) = T_1(2) * D(3) / WL
    CALL RC(CRP32, RP32, CRP, T2)
    CALL RC(CRN32, RN32, CRN, T2)
470 GO TO(550,480,580,580).M
480 GO TO(481,483,485),MY
481 PRINT 482
482 FORMAT(1H06X,2HD26X,1HP8X,1HA9X,6HRF.CF.5X,1HP9X,6HRF.CF.5X,1HN7X,
   14HEN2P5X \cdot 4HEN2I
    GO TO 486
483 PRINT 484
484 FORMAT(1H06X,2HD26X,1HP8X,2HAP8X,2HAS8X,6HRF.CF.5X,1HP9X,6HRF.CF.5
   1X, 1HN7X, 4HEN2R5X, 4HEN2I)
    GO TU 486
485 PRINT 482
486 D2= D2I
    CALL CM(T1,FN2,C2)
500 T2(1)=T1(1)*D2/WL
    T_2(2) = T_1(2) * D_2/WL
    CALL RC(CRP21, RP21, CRP32, T2)
    CALL RC(CRN21,RN21,CRN32,T2)
```

```
CALL CD(RHO, CRP21, CRN21)
    PX=ATN1F(RHO(2),RHO(1))*28.64789-45.
    AX=ATANDF(SQRTF(RHO(1)**2+RHO(2)**2))
    XM1=SQRTF(CRP21(1)**2+CRP21(2)**2)
    THETA1=4TN1F(CRP21(2),CRP21(1))*57.2956
    XM2=SQRTF(CRM21(1)米茶2+CRM21(2) ##2)
    THETA2=ATN1F(CRN21(2),CRN21(1))*57.2956
    GO TO(501,503,505), MY
501 PRINT 502,02,PX,AX,XM1,THETA1,XM2,THETA2, N2(1),FN2(2)
502 FORMAT(1H E9.1,2E9.3,E12.5,E9.3,E12.5,E9.3,2E9.4)
    GO TO 506
503 PXX= .5*ATANDF(SINDF(QWP)*SINDF(2.*PX)/COSPF(2.PX))
    XL = .5*ACOSE(COSDE(2.*PXX)*COSDE(GWP))
    AP = ATANDF(SINDF(AX)*COSF(XL)/ COSDF(AX)/SINF(XL))
    AS = ATANDE(STNDE(AX)*STNE(XL)/COSDE(AX)/COSE(XL))
    PRINT 504, D2, PXX, AP, AS, XM1, THETA1, XM2, THETA2, FN2(1), FN2(2)
504 FORMAT(1H F9+1,3F9+3,F12+5,F9+3,F12+5,F9+3,2F9+4)
    GO TO 506
505 AXX= ATANDF(SINDF(AX)/COSDF(AX)**FN)
    PXX= (PX+45.)*EN-45.
    PRINT 502,02,PXX,AXX,XN1,THETA1,XM2,THETA2,FN2(1),FN2(2)
506 D2 = D2 + DD2
    IF(D2F-D2)520,520,500
520 EN2X(2) = EN2X(2)+DEN2(2)
    IF(FN2F(2)-FN2X(2))530,530,410
530 FN2X(1) = FN2X(1)+DFN2(1)
    FN2X(2) = FN2I(2)
    PRINT 540
540 FORMAT(1H)
    IF(FN2E(1)-FN2X(1))50,50,410
550 CALL SYSTEM
560 RHO(1)=SINDF(A)/COSDF(A)*COSDF(2.*P+90.)
    RHU(2)=SINDF(A)/COSDF(A)*SINDF(2.*P+90.)
    T1(1) = 4 * S1 * 2 RHO(1)
    T1(2)=4.*S1**2*RHO(2)
    T_2(1) = RHO(1) + 1.
    T_2(2) = RHO(2)
    CALL CM(T3,T2,T2)
    CALL CD(T2,T1,T3)
    T_1(1) = 1 - T_2(1)
    T_1(2) = -\Gamma_2(2)
    CALL CSR(T2,T1)
    D(N) = 0.
    FNX(1,N) = S1/C1*T2(1)*FN1
    FNX(2,N) = S1/C1 * T2(2) * FN1
    PRINT 570, FNX(1,N), FNX(2,N), P,A
570 FORMAT(20HOINDEX OF SUBSTRATE=F9.4,F9.4,2H I,2X,2HP=F9.3,2X,2HA=9.
   13)
    GO TO 130
580 RHO(1) = SINDF(A)/COSDF(A)*COSDF(2.*P+90.)
    RHO(2)=SINDF(A)/COSDF(A)*SINDF(2.*P+90.)
    CALL CM(T1,CRN32,CRP32)
    CALL CM(T2,T1,RP21)
    CALL CM(T3,T2,RHO)
    CALL (M(T4,T1,RN21)
```

```
\mathbb{Z}(1) = \mathbb{T}_{3}(1) - \mathbb{T}_{4}(1)
      F(2) = T_3(2) - I_4(2)
      CALL CH(T1,RN21,RP21)
      CALL CM(T2,T1,CRP32)
      T_3(1) = CRN32(1) + T_2(1)
      T_3(2) = CRN32(2) + T_2(2)
      CALL CM(T4,T3,RHO)
      CALL CM(T5,T1,CRN32)
      B(1) = T4(1) - CRP32(1) - T5(1)
      B(2) = T4(2) - CRP32(2) - T5(2)
      CALL CM(T1,RN21,RHO)
      C(1) = T1(1) - RP21(1)
      C(2) = T1(2) - RP21(2)
      CALL CM(T1,B,B)
      CALL CM(T2,E,C)
      T_3(1) = T_1(1) - 4 \cdot * T_2(1)
      T_3(2) = T_1(2) - 4 \cdot * T_2(2)
      CALL CSR(T4,T3)
      DO 590 IX= 1,2
      T1(IX) = -B(IX) + T4(IX)
       T_2(IX) = -B(IX) - T_4(IX)
  590 T3(IX)= 2.*E(IX)
      CALL CD(Y1,T1,T3)
       CALL CD(Y2,T2,T3)
       CALL CM(T1,FN2,C2)
       T3(1)=12.56637*T1(1)/WL
       T3(2)=12.56637*T1(2)/WL
       XX(1) = ATN1F(-Y1(2), Y1(1))
       XX(2)=0.5*LOGF(Y1(1)**2+Y1(2)**2)
       CALL CD(D2C,XX,T3)
       XX(1) = ATN1F(-Y2(2), Y2(1))
       XX(2)=0.5*LOGF(Y2(1)**2+Y2(2)**2)
       CALL CD(D2CX,XX,T3)
       Z=606060606020
R
       IF(ABSF(D2C(2))-ABSF(D2CX(2)))610,610,600
  600 \text{ HOLD} = D2C(1)
       D_{2C(1)} = D_{2CX(1)}
       D2CX(1) = HOLD
       HOLD=D2C(2)
       D2C(2) = D2CX(2)
       D2CX(2) = HOLD
R
       Z=606060606040
  610 D1 = D2C(1)
  620 T2(1) = T1(1)*D1/WL
       T_2(2) = T_1(2) * D_1 / WL
       CALL RC(CRP21, RP21, CRP32, T2)
       CALL RC(CRN21,RN21,CRN32,T2)
       CALL CD(RHO, CRP21, CRN21)
       WP=((FN1**2-1•)/(FN1**2+2•)-(FN2(1)**2-1•)/(FN2(1)**2+2•))*DENP/
      1 (((FN2(1)**2-1•)/(FN2(1)**2+2•))*(DEN1-DENP)-(FNP**2-1•)/
      2 (FNP**2+2•)*DEN1+(FN1**2-1•)/(FN1**2+2•)*DENP)
       DC = WP/(WP/DENP+(1 - WP)/DEN1)*D1*1 - E-5
       ADX = ATANDF(SQRTF(RHO(1) **2 + RHO(2) **2)) - A
       PDX=ATN1F(RHO(2),RHO(1))*28.64789-45.-P
       T_2(1) = T_1(1) * D_2CX(1) / WL
```

```
T2(2)=T1(2)*D2CX(1)/WL
    CALL RC(CRP21, RP21, CRP32, T2)
    CALL RC(CRN21, RN21, CRN32, T2)
    CALL CD(RHO, CRP21, CRN21)
    ADXX=ATANDF(SQRTF(RHO(1)**2+RHO(2)**2))-A
    PDXX=ATN1F(RHO(2),RHO(1))*28.64789-45.-P
    GO TO (625,820,830,880,1030,1190,2030),MX
625 PRINT 630, D1, DC, PDX, ADX, D2C(2), D2CX(1), PDXX, ADXX, D2CX(2), FN2(1),
   1 FN2(2),Z
630 FORMAT(1H F8.1,1PE12.4,0P2F9.3,F12.5,F8.1,2F9.3,F12.5,2F9.5,A6)
    GO TO 520
670 P= Z1
    A = Z2
    AP=Z3
    TNPSI=SQRTF(SINDF(A)/COSDF(A)*SINDF(AP)/COSDF(AP))
    XL=ATN1F(TNPSI,SINDF(A)/COSDF(A))
    QWP=ACOSF(ABSF(COSF(2•*XL)/COSDF(2•*P)))*57•2956
    PRINT 680,QWP
680 FORMAT( 45HORELATIVE RETARDATION OF QUARIER WAVE PLATE = F9.3)
    GO TO 50
810 I=N-2
    PRINT 390.I, FNX(1,N), FNX(2,N), FN, P,A
    FN2X(2) = FN2I(2)
315 FN2(2) = -FN2X(2)
    MX = 2
    X1 = FN2I(1)
    X2 = FN2E(1)
    FN2(1) = X2
    GO TO 420
820 ER2= D2C(2)
    FN2(1) = X1
    MX = 3
    GO TO 420
830 ER1= D2C(2)
    IF(ER1)840,840,850
840 IF(ER2)855,855,870
850 IF(ER2) 870,870,855
855 IF(NCH)856,1031,1031
856 PRINT 857
857 FORMAT(27HONO SOLUTION IN RANGE OF N2)
860 PRINT 630, D1, DC, PDX, ADX, D2C(2), D2CX(1), PDXX, ADXX, D2CX(2), FN2(1),
   1 FN2(2),Z
    GO TO 1020
870 DO 950 I=1,20
    X3 = (X1 + X2)/2.
    FN2(1) = X3
    MX = 4
    GO TO 420
880 ER3 = D2C(2)
    IF(ABSF(PDX)-ABSF(ERP))890,890,900
890 IF(ABSF(ADX)-ABSF(ERA))1170,1170,900
900 IF(ER1)910,910,920
910 IF(ER3)930,930,940
920 IF(ER3)940,940,930
930 X1= X3
```

```
r81= ER3
     GO TU 950
   X2= X3
 14
     ER2=ER3
950 CONTINUE
SOC PRINT 970
970 FURMAT(24MUNO SOLUTIUN IN 20 IRIES)
     GO 10 1030
1020 MX= 5
     FN2(1) = X2
     GO TO 420
1030 PRINT 630.01.0C,PDK,ADX.02C(2).02CK(1).PDYX.AUXX.02CX(2).FN2(1).
    1 FN2(2),Z
1031 EN2X(2)=EN2X(2)+DEN2(2)
     IF(FN2E(2)-FN2X(2))50,50,815
1050 TE(QWP) 1060, 1070, 1060
1066 MY=2
     GO TU 1080
1070 MY=1
1080 IF(FN-1.)1090,320,1050
1090 MY=3,
GO TO 320
1100 P=Z1
     A = Z Z
     IF(QWP)1110,1120,1110
1110 XL=ACOSE(ABSE(COSDE(QWP)*COSDE(2.*P)))/2.
     DEL=ATN1F(SINDF(QWP) - SINDF(2.*P)/COSDF(2.*P))
     A=AIN1F(SINDF(A)/COBEF(A),COSF(XL)/SINF(XL))*57.2956
     AX=ATN1F(SINDF(Z3)/COSDF(Z3)+SINF(XL)/COSF(XL))*57+2956
     PRINT 1115, A, AX
1115 FORMAT(14HOCALCUEATED A=F15.4.4H ANDF15.4)
     P=DEL*28.6478-45.
     A = (A + AX)/2.
1120 IF(FN-1.)1130,1160,1130
1130 TNA=SINDF(A)/COSDF(A)
     IF (TNA) 1140,1150,1150
1140 TNA=-TNA
     P=P+90.
1150 P=(P+45.)/FN-45.
     A=ATANDF(INA**(1./FN))
1160 GO TO (550,550,380,810,560),M
1170 IF(NCH)1175,1030,1175
1175 PRINT 630, D1, DC, PDX, ADX, D2C(2), D2CX(1), PDXX, ADXX, D2CX(2), FN2(1),
    1 FN2(2),Z
     NPCH= XABSE(NCH)
     DO 2011 I=1,NPCH
1180 FN2(1) = FN2(1) - DFN2(1)
     MX = 6
     GO TO 420
1190 IF(ABSF(PDX)-EP)2000,2000,2015
2000 IF(ABSF(ADX)-FA)2010,2010,2015
2010 IF(FN2(1)-FN2I(1))2015,2015,2011
2011 CONTINUE
2015 PRINT 630, D1, DC, PDX, ADX, D2C(2), D2CX(1), PDXX, ADXX, D2CX(2), FN2(1),
    1 FN2(2),Z
```

```
FN2(1)=X3
      DO 2060 I=1,NPCH
 2020 EN2(1)=EN2(1)+DEN2(1)
      MX = 7
      GO TO 420
 2030 IF(APSE(PDX)-EP)2040.2040,1030
 2040 IF(ABSE(ADX)-EA)2050.2050,1030
 2050 IF(FN2(1)-FN2F(1))2060-2060,1030
 2060 CONTINUE
      GO TO 1030
 2070 EP= Z1
      EA = Z2
      GO TO 50
        END
       SUBROUTINE CS(C3,X,FN3)
      DIMENSION C3(2), FN3(2), T1(2), T2(2), T3(2)
      T1(1) = X
      T1(2) = 0.
      CALL CD(T2,T1,FN3)
      CALL CM(T3,T2,T2)
      T1(1) = 1 - T3(1)
      T1(2) = -T3(2)
      CALL CSR(C3,T1)
      X = N1 * SIN(PHI1)
      RETURM
      END
      SUBROUTINE SRC(R, T1, T2)
      DIMENSION R(2), T1(2), T2(2), T3(2), T4(2)
      DO 1 I=1.2
      T_3(I) = T_1(I) - T_2(I)
    1 T_4(I) = T_1(I) + T_2(I)
      CALL CD(R,T3,T4)
      RETURN
      END
      SUBROUTINE RC(CR, RP21, RP32, Q)
С
      MCCRACKIN
                   REFLECTION COEFFICIENT OF A FILM Q=N2*COS(PHI2)*D/WL
      DIMENSION CR(2), RP21(2), RP32(2), Q(2), T1(2), T2(2), T3(2), P(2)
      P(1) = 12.56637 \times Q(1)
      P(2) = 12.56637 \times Q(2)
      T_{2}(1) = E_{XPF}(P(2)) * COSF(P(1))
       T_{2}(2) = -E_{XPF}(P(2)) * SINF(P(1))
      CALL CM(T1,T2,RP32)
      CALL CM(T3,T1,RP21)
       T1(1) = RP21(1) + T1(1)
       T1(2) = RP21(2) + T1(2)
       T_3(1) = 1_{\bullet} + T_3(1)
      CALL CD(CR, T1, T3)
      RETURN
       END
       SUBROUTINE CSR(SRX,X)
       DIMENSION SRX(2),X(2)
С
       SRX=COMPLEX SQRT X, IF SRX(2)=0, SRX(1)=POSITIVE, IF SRX(1)=0,
C
       SRX(2)=NEGATIVE, OTERWISE SRX(1)=POSITIVE AND SRX(2)=CORRECT SIGN
       IF(X(2))4,1,4
    1 \text{ IF}(X(1))2,2,3
```

С

```
2 SRX(1) = 0.
  SRX(2) = -SORTF(ABSF(X(1)))
  GO TU 5
3 SRX(1) = SQRTF(X(1))
  SRX(2) = 0.
  GO TO 5
4 R=SQRTF(X(1)**2+X(2)**2)
  SRX(1) = SQRTF((R+X(1))/2)
  SRX(2) = SIGNF(SQRTF((R-X(1))/2.),X(2))
5 RETURN
  END
  SUBROUTINE CD(T2,T1,T3)
  DIMENSION T1(2), T2(2), T3(2)
  E=T3(1)**2+T3(2)* *2
  T2(1)=(T1(1) *T3(1)+ T1(2)*T3(2))/E
  T_2(2) = (T_1(2) * T_3(1) - T_1(1) * T_3(2)) / E
  RETURN
  END
  SUBROUTINE CM(T3,T1,T2)
  DIMENSION T1(2), T2(2), T3(2)
  T_3(1) = T_1(1) * T_2(1) - T_1(2) * T_2(2)
  T_3(2) = T_1(1) * T_2(2) + T_1(2) * T_2(1)
  RETURN
  END
```

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#### 7. References

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- [4] Proceedings of the Symposium on the Ellipsometer and its Use in the Measurement of Surfaces and Thin Films, National Bureau of Standards, Sept. 5, 6, 1963, to be published by NBS, for sale by the Supt. of Documents, U.S. Government Printing Office, Washington, D. C.
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Fig. 1. Schematic diagram of 5 films on a substrate. Refractive indices of films are  $n_2$  to  $n_6$ , thicknesses of films are  $d_2$  to  $d_6$ , angle of incidence is  $\phi$ , and refractive indices of surrounding medium and substrate are  $n_1$  and  $n_7$ .



Whubers in ovals refer to statement numbers in fortran program. A, B, C, D, DI, and D2 in squares refer to detail dia-grams shown in the following figures. Flow Diagram of Computer Program. . N

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Fig. 4. Diagram C. Calculates and prints ellipsometer readings (PX and Ax or PXX, AP and AS) and reflection coefficients (RP<sub>21</sub> and RN<sub>21</sub>).



TO STATEMENT 1030

Fig. 5. Diagram D. Interprets NCH. If NCH is zero, no calculation is performed, if NCH is not zero, the limits of error for FN2(1) are determined and printed.

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