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# **A Fortran Program for Analysis of Ellipsometer Measurements**



**U.S. DEPARTMENT OF COMMERCE  
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## A Fortran Program for Analysis of Ellipsometer Measurements

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## Contents

	Page
1. Introduction . . . . .	1
2. Data Input Required for Calculations . . . . .	3
2.1. Table of Values for $\Delta$ , $\psi$ , P, A, and Reflection Coefficients for a Film- Covered Surface - CTABLE. . . . .	3
2.2. Optical Constants of a Film-Free Substrate - CNS . . . . .	8
2.3. Input of Ellipsometer Readings, P, A, and Q . . . . .	9
2.4. Corrections to Ellipsometer Readings: ALINE, AT, CAT, CATA. . . . .	10
2.5. Film Thickness for a Film of Known Refractive Index - CD . . . . .	12
2.6. Film Thickness and Refractive Index - CND . . . . .	13
2.7. Confidence Limits of Film Thickness and Refractive Index - CNDE and CNDC. . . . .	15
2.8. Calculations Involving Multiple Films - FILM. . . . .	16
2.9. Inhomogeneous Films - IFILM . . . . .	17
2.10. Multiple Reflections of the Light . . . . .	19
2.11. Films Composed of a Mixture of Materials. . . . .	19
2.12. New Pages, Reset of Variables, and Comments . . . . .	20
2.13. Optical Constants of an Adsorbing Film of Given Thickness - CNK, FT . . . . .	21
3. Theory and Calculations. . . . .	22
3.1. Computation of $\Delta$ and $\psi$ from Ellipsometer Readings. . . . .	22
3.2. Computation of Constants $T_c$ and $\Delta_c$ of the Wave Plate. . . . .	24

	Page
3.3. Computation of the Angle of Tilt of the Reflecting Surface. . . . .	25
3.4. Calculation of the Thickness of a Film from $\Delta$ and $\psi$ . . . . .	27
3.5. Calculation of Both the Refractive Index and Thickness of a Film From Values of $\Delta$ and $\psi$ . . . . .	28
3.6. Confidence Limits for the Refractive Index and Thickness of a Film . . . . .	31
3.7. Volume Fractions and Total Amount of Material for a Film Composed of a Mixture of Two Materials . . . . .	32
3.8. Computation of Ellipsometer Readings from $\Delta$ and $\psi$ . . . . .	33
3.9. Computation of $n$ and $\mu$ of a Film of Given Thickness . . . . .	33
4. The Fortran Program. . . . .	37
4.1. Fortran IV Program. . . . .	38
4.2. Subprograms . . . . .	56
4.3. Variables Used in Program . . . . .	58
a. Variables in Common . . . . .	58
b. Complex Variables Not in Common . . . . .	60
5. References . . . . .	62
Appendix I. Use of the ALINE Instruction in Relation to Alinement of the Ellipsometer. . . . .	64
Appendix II. Derivation of Equation 3 . . . . .	67

# A Fortran Program for Analysis of Ellipsometer Measurements

Frank L. McCrackin

A general Fortran program is given that performs the calculations required to analyze ellipsometer measurements. This program replaces the program given in NBS Technical Note 242, entitled "A Fortran Program for Analysis of Ellipsometer Measurements and Calculation of Reflection Coefficients From Thin Films." The main changes from the previous program are: 1) the new program is in Fortran IV and V rather than Fortran II; 2) the relative transmission of the wave plate is considered in analyzing ellipsometer readings; 3) an improved method is used for calculating the refractive index of a film; 4) the form of the input data is improved; 5) a method for calculating and correcting for tilt of the reflecting surface is given; 6) an improved method of calculating confidence limits for the calculated values of thickness and refractive index of a film is used; and 7) a method for calculating the optical constants of an adsorbing film of given thickness is included.

Key words: Computer programs; ellipsometry; Fortran program; multiple films; optical constants; reflection coefficients; thin films.

## 1. Introduction

The reflection of polarized light from surfaces and thin films has been discussed by various authors [1-4].\* The reflection is expressed in terms of the reflection coefficients  $R^P$  for light polarized parallel to the plane of incidence and  $R^S$  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.

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\*Figures in brackets indicate the literature references on page 62.



The ellipsometer is an optical instrument used to study surfaces and surface films by reflection of light from the surface. The ellipsometer measures the ratio of the reflection coefficients

$$\rho = R^P/R^S = \tan\psi e^{i\Delta}. \quad (1)$$

In the ellipsometer, as considered by this program, monochromatic light passes through a polarizer and a wave plate (linear retarder). It is then reflected from the surface under investigation, and passes through another polarizing prism called an analyzer and to a detector. The wave plate is generally set at a fixed azimuth and the polarizer and analyzer rotated until the light is extinguished as determined by the detector. The azimuths of the polarizer, fast axis of the wave plate, and analyzer, (P, Q, and A), measured from the plane of incidence are recorded. From the reading P, Q, and A,  $\Delta$  and  $\psi$  of eq (1) are first calculated, then the optical constants of the surface or of films on the surface are calculated from  $\Delta$  and  $\psi$ .

In order to calculate  $\Delta$  and  $\psi$  from the ellipsometer readings, the constants of the wave plate must be known. Until recently, the relative phase retardance,  $\Delta_c$ , along the fast and slow axes was believed to describe the optical properties of the wave plate. However, it has been shown [5-8] that the transmissions along the two axes are different. Therefore, the ratio  $T_c$  of the transmission along the fast axis to the transmission along the slow axis of the wave plate must also be considered. In addition, Oldham [6] has shown that a tilt in the mounting of the wave plate can cause  $\Delta_c$  and  $T_c$  to vary with the azimuth of the wave plate. This program takes both  $\Delta_c$  and  $T_c$  and their variation with Q into consideration in computing  $\Delta$  and  $\psi$ . The values of  $\Delta_c$  and  $T_c$  may also be computed from the ellipsometer readings.

Another possible source of error is a tilt of the reflecting surface. The instrument is aligned so that P, Q, and A are read with respect to the reflecting surface. If the reflecting surface is changed, and the new surface is tilted with respect to the



surface with which the ellipsometer was aligned, the readings of P, Q, and A will be in error. This error could be eliminated by re-alignment, but this is time consuming. Therefore, the program has been written to calculate the angle of tilt from the ellipsometer readings and correct for the tilt.

## 2. Data Input Required for Calculations

The data and instructions are given to the computer by punched cards. Each card requires an instruction starting in column 1. The data required for the instruction start in columns 10, 20, 30, 40, 50, and 60. All numbers must contain a decimal point.

Instructions that start with C cause the computer to perform calculations. These instructions are listed in table 1. The other instructions are used to give data for future calculations. Table 2 gives the required data with each instruction.

### 2.1. Table of Values for $\Delta$ , $\psi$ , P, A, and Reflection Coefficients for a Film-Covered Surface - CTABLE

The instruction CTABLE will produce calculation of ellipsometer readings and reflection coefficients for reflection of light from a film-covered surface. The thickness of the film is given on the same card as the instruction. However, before the CTABLE instruction is given, instructions NM, NF, NS or CNS, AI, and WL (see table 2) must be used to give values of the refractive index of the medium, film, and substrate and the angle of incidence and wave length of the light, respectively. For example,

1	10	20	30	40
NM	1.			
NF	1.4			
NS	1.7			
AI	65.			
WL	4800.			
CTABLE	40.			

Table 1. Computations

Instruction	Computes	Preceding Instructions Required If Standard Values Are Not Used
CAT	Angle of tilt of reflecting surface	WP or CWP
CD	Thickness of film	NM, NF, NS or CNS, AI, NREF, WL <sup>1</sup>
CND	Refractive index and thickness of film	NM, NF, NS or CNS, AI, NREF, WL, ELDP <sup>1</sup>
CNDC	Refractive index and thickness of film with allowed combination of values	NM, NF, NS or CNS, AI, NREF, WL, ELDP, EDP <sup>1</sup>
CNDE	Refractive index and thickness of film with confidence limits	NM, NF, NS or CNS, AI, NREF, WL, ELDP, EDP <sup>1</sup>
CNK	Refractive index and $n$ of film of given thickness	NM, NF, NS or CNS, AI, NREF, WL, FT <sup>1</sup>
CNS	Refractive index of substrate	NM, AI, NREF <sup>1</sup>
CTABLE	Table of $\Delta$ and $\psi$ and reflection coefficients	NM, NF, NS or CNS, AI, NREF, WL
CWP	Constants $T_c$ and $\Delta_c$ of wave plate	None

<sup>1</sup>Instructions WP or CWP required if ellipsometer readings (P, A, and Q) are given.

Table 2. Data Given With Instructions

Card Column No.						
1	10	20*	30	40	50*	60
AI	$I(\varphi)$	$\delta(\varphi)$	$E(\varphi)$			
ALINE	$\Delta P$	$\Delta A$	$\Delta Q$			
AT	Angle					
CAT	$P_1$	$A_1$	$P_2$	$A_2$	Q	
CATA	$P_1$	$A_1$	$P_2$	$A_2$	Q	
CD	}					
CND		$\Delta$	$\psi$			
CNDC		P	A	Q		
CNDE		$P_1$	$A_1$	$P_2$	$A_2$	Q
CNK		blank				
CNS						
CTABLE	$I(d)$	$\delta(d)$	$E(d)$	$Q^{**}$		
CWP	$P_1$	$A_1$	$P_2$	$A_2$	Q	
EDP	$E\Delta$	$E\psi$				
ELDP	$E\Delta$	$E\psi$				
FILM	No.	d	n	$\kappa$		
FT	$I(d)$	$\delta(d)$	$E(d)$			
IFILM	No. films	d	$n_{top}$	$\kappa_{top}$	$n_{bottom}$	$\kappa_{bottom}$
MIXED	$\rho_1$	$\rho_p$	$n_p$			
NF	$I(n)$	$\delta(n)$	$E(n)$	$I(\kappa)$	$\delta(\kappa)$	$E(\kappa)$
NM	$I(n)$	$\delta(n)$	$E(n)$			
NREP	No. Reflections					
NS	$I(n)$	$\delta(n)$	$E(n)$	$I(\kappa)$	$\delta(\kappa)$	$E(\kappa)$
PAGE	See Section 2.12					
RESET	See Section 2.12					
STØP						
WL	$I(\lambda)$	$\delta(\lambda)$	$E(\lambda)$			
WP	$T_c$	$\Delta_c$				
(other)	Comment					

\* The symbol  $\delta$  refers to incremental values.

\*\*The value of Q with this instruction is optional. See Section 2.1.

Table 3. Assigned Values

Symbol	Data	Instruc- tion	Assigned Values
$N_n$	Index of medium	NM	1
$N_2$	Index of film	NF	1
$N_s$	Index of substrate	NS	1
$\phi_1$	Angle of incidence	AI	70°
$\lambda$	Vacuum wavelength of light	WL	5461
$T_c, \Delta_c$	Constants of wave plate	WP	1, 90°
	Number of reflections of light	NREF	1
	Experimental errors of $\Delta$ and $\psi$	EDP	.015, .015
	Error limits of $\Delta$ and $\psi$ used for computing $n_2$	ELDP	.002, .002
	Angle of tilt	AT	0

will compute  $\Delta$  and  $\psi$  and reflection coefficients for the condition:

Refractive index of medium = 1.  
 Wave length of light = 4800. Å  
 Angle of incidence = 65.°  
 Thickness of film = 40. Å  
 Refractive index of film = 1.4  
 Refractive index of substrate = 1.7

A range of values of the input parameters may also be specified by giving the initial value, increment, and final value to be used. Thus, the input data

<u>1</u>	<u>10</u>	<u>20</u>	<u>30</u>	<u>40</u>
NM	1.			
NF	1.4	0.1	1.6	
NS	1.7			
AI	65.			
CTABLE	0.	20.	100.	

will produce tables for films of refractive index of 1.4, 1.5, and 1.6. In each table, the ellipsometer readings and reflection coefficients will be given for films 0, 20, 40, 60, 80, and 100 Å thick. The results are given in the upper portion of figure 1. The other parameters may also be similarly varied.

In this figure the values of  $\Delta$  and  $\psi$  for the sample, then the complex reflection coefficients for light polarized parallel and normal to the plane of incidence, are printed. For the complex reflection coefficients, the ratios of reflected to incident amplitudes and the change in degrees of the phase of the light are given. The intensity ratios for parallel and normally polarized light are the squares of the corresponding amplitude ratios.

The refractive index and value of  $\kappa$  for the film and substrate are next printed. In this example, the film and substrate are non-absorbing so the values of  $\kappa$  are zero.



A setting, Q, for the wave plate starting in column 40, may also be given with the CTABLE instructions. In this case, the two sets of ellipsometer readings, P1,A1 and P2,A2, (see Section 2.3) that will produce extinction of the light are also calculated and printed, as shown in figure 1.

Listed in table 3 are values for certain of the input parameters. These assigned values are automatically used for following calculations unless instructions are given to change them. Thus, in the above examples, the NM instruction was not necessary as the assigned value of 1, was used for the index of the medium.

The film or substrate may also be absorbing. In this case the optical constants are  $n$  and  $\kappa$  of the complex refractive index  $n - n\kappa i$ . The values of  $n$  and  $\kappa$  are given starting in columns 10 and 40. Thus, the card

Column No.				
1	10	20	30	40
NS	3.316			1.4

defines an absorbing substrate with  $n=3.316$  and  $\kappa=1.4$  or of complex refractive index of  $3.316(1-1.4i)$ .

The value of  $n$  may be varied by giving the initial, incremental, and final values starting in columns 10, 20, and 30, and  $\kappa$  may be varied by giving the initial, incremental, and final values starting in columns 40, 50, and 60.

## 2.2. Optical Constants of a Film-Free Substrate - CNS

The instruction CNS calculates the optical constants  $n_s$  and  $\kappa_s$  of a substrate from measurements of  $\Delta$  and  $\psi$  for the substrate without a film. The values of  $\Delta$  and  $\psi$  start in columns 10 and 20 of the card containing CNS. The values of  $n_s$  and  $\kappa_s$  are printed and also retained by the computer so they will be used in following calculations, such as CTABLE, for which they are required. Thus, the optical constants of the substrate may be given by either an NS or CNS instruction.



Ellipsometer readings of P, A, and Q, rather than values of  $\Delta$  and  $\psi$  may be used with the CNS instruction, as explained in the next section.

### 2.3. Input of Ellipsometer Readings P, A, and Q

As previously described, the ellipsometer readings must first be analyzed to obtain the values of  $\Delta$  and  $\psi$  that describe the reflection of the light from the surface before the instruction CNS, or the instructions CD, CND, CNDC, CNDE to be later described, may be used. However, the ellipsometer readings may also be used as input data with these instructions if the components of the ellipsometer are arranged in the order of light source, polarizer, wave plate, reflecting surface, analyzer, and detector.

Let the wave plate be set with its fast axis at an azimuth Q and let extinction of the light be obtained with the polarizer and analyzer at azimuths P and A (see Reference 4). All azimuthal angles are measured positive counterclockwise from the plane of incidence. Then these readings of P, A, and Q may be used with the above instructions, as shown in table 2. The computer first calculates the values of  $\Delta$  and  $\psi$  and uses them in the following calculations.

Let  $P_1$  and  $A_1$  be settings of the polarizer and analyzer that produce extinction of the light for a given value of Q. Then, settings of for example  $P_1 + 180^\circ$ ,  $A_1$ ;  $P_1$ ,  $A_1 + 180^\circ$ ; and  $P_1 + 180^\circ$ ,  $A_1 + 180^\circ$  produce the same effect on the polarized light so will also give extinction. That is, P and A are indeterminate to  $\pm 180^\circ$ . This duplication of settings may be eliminated by, for example, taking only P and A readings between 0 and  $180^\circ$ . After eliminating duplicate readings, two sets of readings  $P_1, A_1$  and  $P_2, A_2$  will be found to give extinction for a given setting Q of the wave plate. Both sets of readings may be used with the instructions CD, CND, CNDE, and CNS. They are given in the order  $P_1, A_1, P_2, A_2, Q$ .

The computer calculates values of  $\Delta$  and  $\psi$  from each set of readings and uses the averages of them in the following calculations.

In order for the computer to calculate  $\Delta$  and  $\psi$  from the ellipsometer readings, the constants of the wave plate must have been previously made available to the computer. The constants are the ratio,  $T_c$ , of the transmittance of the wave plate along the fast axis to the transmittance along the slow axis and the phase retardance along the fast axis minus the phase retardance along the slow axis,  $\Delta_c$ . They may be given in the order  $T_c$ ,  $\Delta_c$  with the instruction WP or may be calculated from a set of readings  $P_1$ ,  $A_1$ ,  $P_2$ ,  $A_2$  and Q by the CWP instruction.

More than one calculation may be performed with a single set of ellipsometer readings. In this case, a set of ellipsometer readings from a film-free metal surface is used to first calculate the constants of the wave plate by the CWP instruction, and then is used to calculate the optical constants of the metal by the CNS instruction. The readings do not have to be repeated with the CNS instruction.

#### 2.4. Corrections to Ellipsometer Readings:

##### ALINE, AT, CAT, CATA

The ellipsometer angular readings of P, A, and Q must sometimes be corrected to obtain angles measured from the plane of incidence of the reflection from the surface, as is required for this program. For example, if a dial reads from the plane of the surface,  $90^\circ$  must be added to the dial readings. As another example, in alining the ellipsometer the dial readings when the component is alined in the plane of incidence may be recorded and used as a correction to future readings of the dial, rather than adjusting the dial or the vernier on the dial to read correctly. This method of alinement is described in Appendix I.

The corrections ( $\Delta P$ ,  $\Delta A$ , and  $\Delta Q$ ) may be given by the ALINE Instruction (see table 2). Then the corrections will be added to values of P, A, and Q given with all following instructions.

A correction to the ellipsometer readings may also be required due to tilting of the reflecting surface. This may occur when the ellipsometer is alined with one surface, and then the surface is replaced by another surface that is to be measured. The second surface may be tilted with respect to the orientation of the first surface so the ellipsometer will no longer be properly alined but all its readings must be corrected by the angle of tilt. This correction may be given to the computer by the AT instruction. The AT instruction differs from the ALINE instruction in that one correction is given to be added to all values of P, A, and Q, while different corrections for P, A, and Q are given with the ALINE instruction.

The angle of tilt of the reflecting surface is generally unknown. It may be computed from ellipsometer readings by the instruction CAT. The instruction CAT requires the two sets of P and A readings for a setting of Q and the constants  $T_c$  and  $\Delta_c$  of the wave plate. The calculated value of the angle of tilt will be added to all ellipsometer readings given by following instructions.

The theory of this calculation is given in Section 3.3. This theory requires that the angle of tilt is small. The calculation has been found to be accurate for angles of tilt up to one degree.

The constants of the wave plate may not be calculated from the same readings used to compute the angle of tilt, since readings from an untilted surface are required to compute the wave plate constants. The usual procedure is to aline the ellipsometer and calculate the constants of the wave plate from ellipsometer readings. Then, every time the surface is changed, its angle of tilt is calculated using the previously determined constants of the wave plate. The angle of tilt of the surface is then used to correct all ellipsometer readings obtained using the surface.



Often two sets of ellipsometer readings are taken for the same surface. For example, readings may be taken for two readings of Q or readings may be taken both before and after a film forms on the surface. Values for the angle of tilt of the surface may be calculated by the instruction CAT for both sets of readings and should be nearly equal. However, subsequent ellipsometer readings will be corrected by the angle of tilt calculated by the last CAT instruction, while for greatest accuracy, the average of the angles computed by the two CAT instructions should be used. This is accomplished by using the instruction CATA to compute the second angle of tilt. The instruction CATA performs the same calculations as CAT, then averages the computed and previously computed values of the angle of tilt. Subsequent ellipsometer readings will then be corrected by the average angle of tilt.

#### 2.5. Film Thickness for a Film of Known Refractive Index - CD

The instruction CD computes the thickness of a film from values of  $\Delta$  and  $\psi$ . The ellipsometer readings P, A, and Q may also be used as described in the previous section. Before this instruction is used, the following data must have been previously given to the computer or standard values will be used:

- 1) Wave Length of Light by instruction WL
- 2) Angle of Incidence by instruction AI
- 3) Refractive Index of Film by instruction NF
- 4) Refractive Index of Substrate by instruction NS or CNS
- 5) Refractive Index of Medium by instruction NM.

If ellipsometer readings are given, the wave plate constants must also be given by instruction WP or CWP, or the standard values will be used.

For example, suppose a film-free surface was measured under water (refractive index of 1.33) with a perfect quarter wave plate set with its fast axis at  $45^\circ$  from the plane of incidence. Let the values obtained be  $P = 86.35$ ,  $A = 25.19$  and  $P = 176.35$ ,  $A = 154.81$  for the two zones. Then let an absorbing film of refractive index  $2.5(1-0.3i)$  be placed on the surface and measurement  $P = 94.30$ ,  $A = 24.44$  be obtained in one zone. Let the angle of incidence be  $65^\circ$  and the vacuum wavelength of the light be  $5461 \text{ \AA}$ . Then the following input data will calculate the refractive index of the substrate and the thickness of the film.

	Column No.				
1	10	20	30	40	50
NM	1.33				
NF	2.5			0.3	
AI	65.				
CNS	86.35	25.19	176.35	154.81	45.
CD	94.30	24.44	45.		

Notice that the wavelength is not given since its assigned value is used. The computer output is shown in figure 2.

## 2.6. Film Thickness and Refractive Index - CND

The instruction CND calculates both the thickness and refractive index of a film from ellipsometer measurements  $\Delta$  and  $\psi$  or from ellipsometer readings  $P$ ,  $A$ , and  $Q$ . The data given to the computer before this instruction is the same as for the CD instruction. However, values for the refractive index of the film given by the NF instruction do not have their usual meaning. Consider first the case that the film has a real refractive index (non-absorbing film). Then the CND instruction causes the computer to search for the refractive index of the film between the limits of the initial value and the sum of the initial and increment values.

Then the search is repeated between the sum of the initial value and increment and the sum of the initial value and twice the increment. This is continued until the final value is reached. For example, if the instruction

```
NF          1.4      .1      1.6
```

is followed by a CND instruction, the computer will search for values of  $n_f$  between 1.4 and 1.5, and between 1.5 and 1.6. If the increment is not given, the computer will perform a single search between the initial and final values.

The search procedure is explained in section 3.5. The limits of film refractive index given by the NF instruction must be chosen with care. If the limits do not include the solution for the film refractive index, the solution will not be found. On the other hand, if the limits are too broad, a solution may be missed.

An example of instruction CND is given in figure 3. In this example, the values of  $\Delta$  and  $\psi$  are given with the instruction CND. The solution of a film of refractive index of 1.2 and thickness of 1000 Å is found. This solution reduces the error terms  $\Delta\text{DEL}$ ,  $\Delta\text{PSI}$ , and  $\text{ERROR}$  to be essentially zero. The terms labeled  $\text{ADSORPTION}$  and  $\text{WT FRACTION}$  have no meaning since the instruction  $\text{MIXED}$  was not given (see 2.11). For the meaning of  $K$ , see section 4.3.

Consider next the case that the film is absorbing but its value of  $n$  is known. Therefore, only the real part of the refractive index and the thickness of the film are to be determined. In this case the imaginary part of the refractive index of the film is given, starting in column 40 of the NF instruction card and the calculations are the same as the previous case.

In the most difficult case, the film is absorbing and both the real and imaginary part of its refractive index as well as its thickness are to be determined. For this case the range of values of the imaginary part is given by the NF instruction and the real



part of the index and thickness of the film is calculated for each value. Thus, the instructions

Column No.

1	10	20	30	40	50	60
NF	1.0		2.0	0.	0.1	1.
CND	152.30	29.00				

will compute the real part of the refractive index and thickness of the film for assumed values of the imaginary part of the refractive index of 0, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, and 1. The real part of the refractive index is assumed to lie between 1. and 2.0. In order to determine which of the calculations correspond to the actual film, additional information is required. Obviously, three values describing the film cannot be determined from the two ellipsometer measurement  $\Delta$  and  $\psi$ . For example, if the thickness of the film was known independently of the ellipsometer readings, the refractive index of the film can be read from the calculations. Other possible methods of determining the refractive index of adsorbing films have been given by McCrackin and Colson [9].

2.7. Confidence Limits of Film Thickness  
and Refractive Index -  
CNDE and CNDC

The instruction CNDC performs the same calculations as instruction CND discussed in the previous section and, in addition, computes limits of error for the calculated refractive index corresponding to the experimental errors in the ellipsometer measurement  $\Delta$  and  $\psi$ . The experimental errors,  $E\Delta$  and  $E\psi$  in  $\Delta$  and  $\psi$  must have been previously given by an EDP instruction or their standard values of  $0.015^\circ$  are used. This instruction is illustrated in figure 4.

The 95% confidence limits of the experimental errors based on a large number of degrees of freedom must be used for  $E\Delta$  and  $E\psi$ . That is, the true value of  $\Delta$  lies in the range  $\Delta - E\Delta$  to  $\Delta + E\Delta$  with 95% probability, and likewise for  $\psi$ . An ellipse is then calculated such that the true values of  $\Delta$  and  $\psi$  will lie within it with 95% probability. Figure 5 shows the ellipse for the conditions of figure 4. (When the errors are equal, this ellipse becomes a circle.)

After calculating the best values for the refractive index  $n_f$  and the thickness  $d_f$  of the film from the measured  $\Delta$  and  $\psi$  readings, the computer chooses eight evenly-spaced pairs of values from the probability ellipse and computes values of  $n_f$  and  $d_f$  for each pair. An example is shown in figure 4. The best way to represent these values is to plot  $n_f$  versus  $d_f$  as shown in figure 6. The points define a curve (approximately an ellipse) surrounding the best value. The true values of  $n_f$  and  $d_f$  lie within this curve with 95% probability.

This error analysis only takes the errors in the ellipsometer readings into account. Other errors, such as errors in the refractive indexes of the medium and substrate, errors in the angle of incidence, etc., will, of course, increase the error in the calculated values of  $n_f$  and  $d_f$ .

## 2.8. Calculations Involving Multiple Films - FILM

The calculations previously described may also be performed for a number of films on the substrate. Three films on a substrate are represented in figure 7. In order to compute the values of  $\Delta$  and  $\psi$  for reflection from this surface, the optical constants and thickness of the three films and the optical constants of the medium and substrate must be given. The films are numbered starting from the surrounding medium. The optical constants of the surrounding medium, film no. 1, and the substrate are given by NM, NF, and NS or CNS instructions as previously described. The thickness of film

number 1 is treated in the same way as previously described for a single film, i.e., it is given with the CTABLE instruction when the CTABLE instruction is used, or is calculated by the CD, CND, CNDE, or CNDC instructions. The optical constants and thicknesses of the films are given by the FILM instruction. With this instruction: FILM starts in column 1, the number of the film starts in column 10, the thickness of the film in column 20, and the optical constants of the film,  $n$  and  $\kappa$ , start in columns 30 and 40. Up to 900 films may be specified.

## 2.9. Inhomogeneous Films - IFILM

All the previously described computations are for homogeneous films, i.e., films for which the optical constants are the same at all points in the film. However, inhomogeneous films for which the optical constants vary along the thickness of the film may be accurately approximated by multiple homogeneous films [9] by use of the instruction FILM described in the previous section. To illustrate, consider a film 100 Å thick whose optical constants vary from  $n=1$ ,  $\kappa=0$  adjacent to the surrounding medium to  $n=3$ ,  $\kappa=1.4$  adjacent to the substrate. Let the variation be linear with distance. Then the film may be approximated by 10 homogeneous films as shown in figure 8. Let the optical constants of the substrate be  $n=3$  and  $\kappa=1.4$  and the other parameters of the system have their standard values. Then the reflection coefficients and  $\Delta$  and  $\psi$  for reflection from the film are calculated by the instructions given below.

	Column No.			
1	10	20	30	40
NS	3.			1.4
NF	1.1			.07
FILM	2.	10.	1.3	.21
FILM	3.	10.	1.5	.35
FILM	4.	10.	1.7	.49
FILM	5.	10.	1.9	.63
FILM	6.	10.	2.1	.77
FILM	7.	10.	2.3	.91
FILM	8.	10.	2.5	1.05
FILM	9.	10.	2.7	1.19
FILM	10.	10.	2.9	1.33
CTABLE	10.			

The results are shown in figure 9. Approximating this inhomogeneous film with 60 homogeneous films gives  $\Delta=117.625^\circ$  and  $\psi=30.852^\circ$ . Thus, approximating this inhomogeneous film by 10 homogeneous films gave results accurate to  $0.1^\circ$  in this case.

The amount of input data for this type of calculation may be reduced by using the instruction IFILM. The data given with IFILM are the number of homogeneous films to be used to represent the inhomogeneous film, the thickness of the inhomogeneous film, the optical constants of the surface and the inhomogeneous film in contact with the immersion medium, and the optical constants of the surface of the film in contact with the substrate. However, film number 1 (the film next to the surrounding medium) is not assigned a thickness or optical constants by IFILM. Thus, the previous calculation may be obtained from the data:

	Column No.					
1	10	20	30	40	50	60
NS	3.		1.4			
NF	1.					
IFILM	10.	100.	1.	0.	3.	1.4
CTABLE	0.					



The inhomogeneous film is represented by films 2 to 11. Film number 1 is given zero thickness so has no effect on the results. The values given with IFILM are the number of homogeneous films used to approximate the inhomogeneous film, the thickness of the inhomogeneous film, the values of  $n$  and  $\mu$  at the top (next to surrounding medium) of the inhomogeneous film, and the values of  $n$  and  $\mu$  at the bottom (next to substrate) of the inhomogeneous film, respectively. (See table 2, page 5.) Note that all data, including the number of films, must contain a decimal point.

#### 2.10. Multiple Reflections of the Light

The sensitivity of ellipsometer readings to a thin film on a reflecting surface may be increased by reflecting the light from the surface a number of times. An example of this technique, as well as a discussion of the increase of sensitivity, has been given by Stromberg, Passaglia, and Tutas [10]. To analyze such results the number of reflections may be entered, starting in column 10, on a NREP instruction. The number of reflections must have a decimal point even though it is an integer. All following calculations will then be performed for multiple reflection of the light.

Notice that this instruction is not necessary for the multiple reflections of the light that occur from the surfaces of multiple films, but only for the case that the light emergent from reflection from the surface is again incident on and reflected from the surface.

#### 2.11. Films Composed of a Mixture of Materials

In some applications of ellipsometry, the film being studied is a mixture of a material with the medium above the film. For example, polymer films adsorbed from a solvent on a solid surface [10]

consist of a mixture of the polymer and solvent. As another example, a rough clean substrate may be approximated by the system of the substrate, a film consisting of a mixture of the substrate and the medium, and the medium. For these applications, after the refractive index of the film,  $n_f$ , is determined by ellipsometry, the fraction of the film composed of the material and the amount of material per unit area of the surface is desired. These quantities are computed by the instructions CD, CND, CNDC, and CNDE. The amount of the material per unit area of the surface in units of  $\text{mg}/\text{cm}^2$  is printed in the column labeled ADSORPTION and the weight fraction of material in the film is printed in the column labeled WT FRACTION.

In order for these calculations to be meaningful, the density of the medium,  $\rho_1$ , the density of the material in the film,  $\rho_p$ , and the refractive index,  $n_p$ , of the material in the film must have been previously given by the instruction MIXED (see table 2 on page 5). The refractive index of the material in the film of the medium are assumed to be real.

The calculations are described in Section 3.

#### 2.12. New Pages, Reset of Variables, and Comments

The instruction PAGE will start a new page of output. For the Fortran V version of the program, comments may be punched in columns 10 to 80 on the same card and will appear on the new page of output. For the Fortran IV version, the comment must be punched on a card following the card containing the instruction PAGE. For this case, any location on the card is satisfactory.

The instruction RESET has the same function as the instruction PAGE and in addition resets all the parameters to the values given in table 3. This instruction placed between two sets of calculations insures that none of the data given for the first set will be used in the second set of calculations.



In addition, for the Fortran V version of the program, any card that does not contain one of the instructions listed in table 2 starting at the first column of the card will be printed as a comment. Therefore, comments may be freely interpreted with the data cards. For the Fortran IV version of the program, comments can only be inserted following a PAGE or RESET instruction.

The instruction ~~STOP~~ is placed at the end of the program.

### 2.13. Optical Constants of an Adsorbing Film of Given Thickness - CNK, FT

The instruction CNK computes values of  $n$  and  $\kappa$  of a film from ellipsometer readings. Values of  $\Delta$  or  $\psi$  or the ellipsometer readings are given with the CNK instruction in the same way as described in section 2.3 for instructions CD, CND, etc. The instruction CNK must be preceded by instructions FT, NF, and NS or CNS. Also, CWP or WP must be given if ellipsometer readings are given with the CNK instruction and NM, AI, and WL instructions if values other than the assumed values are to be used for the refractive index of the medium, the angle of incidence, and the wavelength of the light.

The instruction FT gives the thickness or thicknesses of the film for which the optical constants are to be calculated. The values given with the FT instruction are the same as for the CTABLE instruction (table 2).

The values given with the NF instruction give the ranges in which the computer will search for values of  $n$  and  $\kappa$  that correspond to the given ellipsometer measurements. Multiple solutions may be found, in which case, means other than the ellipsometer measurements must be used to choose the correct solution. The incremental values for  $n$  and  $\kappa$  given with the NF instruction determine the fineness of the search for the values of  $n$  and  $\kappa$ . If two solutions for  $n$  and  $\kappa$  exist, the  $n$  values or  $\kappa$  values must differ by more than the incremental values for both solutions to be found.

An example of these instructions is given in figure 10. The assumed values are used for the index of the medium, angle of incidence, and wavelength of light. For every given value of film thickness, three solutions for  $n$  and  $\kappa$  (NF and KAPPA) are found in this example. The accuracy to which they are determined is given in the  $\Delta NF$  and  $\Delta KAPPA$  columns.

Thus, for these data, the exact solutions of  $n$  and  $\kappa$  may differ by up to .0002 and .00002, respectively, from the solutions given.

For each solution of  $n$  and  $\kappa$  and each film thickness, values of  $\Delta$  and  $\psi$  are calculated. The differences between these calculated values and the values given with the CNK instruction are given in the  $\Delta DELTA$  and  $\Delta PSI$  columns. These values shall be less than the inaccuracies of the given values of  $\Delta$  and  $\psi$  for the solution to be satisfactory. If  $\Delta$  and  $\psi$  are correct to  $0.01^\circ$ , some of the solutions, for example the first solution, are not satisfactory. These data could be rerun with smaller incremental values for  $n$  and  $\kappa$  on the NF instruction in order to locate the solutions more accurately.

### 3. Theory and Calculations

The theory of the ellipsometer has been given by various investigators [1-8]. Therefore, only special points of the theory necessary to understand the calculations performed by this program will be given.

#### 3.1. Computation of $\Delta$ and $\psi$ From Ellipsometer Readings

Let  $P$ ,  $A$ , and  $Q$  be the azimuths of the polarizer, analyzer, and wave plate, respectively, for extinction of the light by the ellipsometer. For the calculations described in this section, the components of the ellipsometer must be arranged in the order of light source, polarizer, wave plate, reflecting surface, analyser,

and light detector. All azimuths are measured counter-clockwise from the plane of incidence looking into the light beam.

The wave plate is characterized by the ratio,  $T_c$ , of the transmittance along its fast axis to the transmittance along its slow axis\* and the relative phase retardation,  $\Delta_c$ , along the axes. In the following equation it is characterized by the complex number

$$\rho_c = T_c \exp(-i\Delta_c) = T_c \cos\Delta_c - iT_c \sin\Delta_c \quad (1)$$

that has been previously computed. The surface is characterized by the complex value

$$\rho = R_p/R_s = \tan\psi \exp(i\Delta) \quad (2)$$

where  $R_p$  and  $R_s$  are the complex reflection coefficients for light polarized parallel and normal to the plane of incidence of the light beam. The value of  $\rho$  is to be calculated from readings P, A, and Q, and  $\rho_c$ . This calculation is based on the formulas derived by Holmes and Feucht [7]. Modifying their equations 19 and 21 for the conventions used in this report for measurement of P, A, and Q gives

$$\rho = \frac{\tan A [\tan Q + \rho_c \tan (P-Q)]}{\rho_c \tan Q \tan (P-Q) - 1} \quad (3)$$

for extinction of the light. A derivation of eq (3) is also given in Appendix II.

$\Delta$  and  $\psi$  are computed from eqs 1 through 3. If two sets of values of P and A are given,  $\rho$  is computed for each set and the average of the two values used to compute  $\Delta$  and  $\psi$ .

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\* When the previous program was written, the importance of  $T_c$  in ellipsometry was not recognized, thus no correction for it was included in the calculations.

### 3.2. Computation of Constants $T_c$ and $\Delta_c$ of the Wave Plate

For computation of the constants of the wave plate, two sets of readings of P and A ( $P_1$  and  $A_1$  and  $P_2$  and  $A_2$ ), that produce extinction of light for the same value of Q are required. Then, by eq 3

$$\rho = \frac{\tan A_1 [\tan Q + \rho_c \tan (P_1 - Q)]}{\rho_c \tan Q \tan (P_1 - Q) - 1}$$

$$= \frac{\tan A_2 [\tan Q + \rho_c \tan (P_2 - Q)]}{\rho_c \tan Q \tan (P_2 - Q) - 1} \cdot$$

Solving for  $\rho_c$  gives

$$\rho_c = \frac{B \pm j [-B^2 - \tan (P_1 - Q) \tan (P_2 - Q)]^{\frac{1}{2}}}{-\tan (P_1 - Q) \tan (P_2 - Q)} \quad (4)$$

where

$$B = \frac{\tan A_1 [\tan (P_2 - Q) \tan Q - \tan (P_1 - Q) / \tan Q]}{2 (\tan A_1 - \tan A_2)}$$

$$- \frac{\tan A_2 [\tan (P_1 - Q) \tan Q - \tan (P_2 - Q) / \tan Q]}{2 (\tan A_1 - \tan A_2)} \cdot \quad (5)$$

Using eq 1 we find

$$T_c = \frac{1}{\pm [-\tan (P_1 - Q) \tan (P_2 - Q)]^{\frac{1}{2}}} \cdot \quad (6)$$

Since  $T_c$  is real and positive,  $\tan (P_1 - Q) \tan (P_2 - Q)$  must be negative and the plus square root is used. Also,

$$\tan \Delta_c = \frac{\pm [-B^2 - \tan (P_1 - Q) \tan (P_2 - Q)]^{\frac{1}{2}}}{B} \cdot \quad (7)$$



$\Delta_c$  is defined as the phase of light transmitted along the fast axis of the wave plate minus the phase of light transmitted along its slow axis. Therefore,  $0 \leq \Delta_c \leq 180^\circ$ , so  $\sin \Delta_c$  is positive.

Then, by eq 1, the imaginary part of  $\rho_c$  is negative. This requires the negative sign for the imaginary term in eq 4 to be used since the denominator has been shown to be positive. Thus,

$$\tan \Delta_c = \frac{+[-B^2 - \tan (P_1-Q) \tan (P_2-Q)]^{\frac{1}{2}}}{B} . \quad (8)$$

### 3.3. Computation of the Angle of Tilt of the Reflecting Surface

For this calculation, the reflecting surface is assumed to be rotated through a small angle  $\delta$  around an axis of the intersection of the specimen and the plane of incidence. This rotation or tilting of the specimen has many effects. The angle of incidence to the surface will be changed, but by a negligible amount for small angles of tilt. The direction of the reflected light beam will be changed but is assumed to still pass through the apertures in the instrument. The main effect will be a reading error of the azimuths of the polarizer, analyzer, and wave plate. Since these elements are aligned with respect to the reflecting surface, a tilt of the surface by an angle  $\delta$  will change the readings of these azimuths by  $\delta$ . That is

$$\begin{aligned} P_1 &= P_1' + \delta & P_2 &= P_2' + \delta \\ A_1 &= A_1' + \delta & A_2 &= A_2' + \delta \\ Q &= Q' + \delta \end{aligned} \quad (9)$$

where  $P_1'$ ,  $A_1'$ ,  $P_2'$ ,  $A_2'$ , and  $Q'$  are readings of the azimuths and  $P_1$ ,  $A_1$ ,  $P_2$ ,  $A_2$ , and  $Q$  are the true azimuths that would be measured by a properly aligned instrument.

By eq 3, for the first set of readings

$$\rho = \frac{\tan (A_1' + \delta) [\tan (Q' + \delta) + \rho_c \tan (P_1' - Q')]}{\rho_c \tan (Q' + \delta) \tan (P_1' - Q') - 1} . \quad (10)$$

The tangents are expanded in  $\delta$  and only the term in  $\delta$  retained, since  $\delta$  is small.

$$\begin{aligned} \tan (A_1' + \delta) &\cong \tan A_1' + \delta / \cos^2 A' \\ \tan (Q' + \delta) &\cong \tan Q' + \delta / \cos^2 Q' \end{aligned} \quad (11)$$

Eqs 11 are substituted in eq 10 and the result simplified to give

$$\rho = \frac{\alpha_1 + \beta_1 \delta}{\gamma_1} \quad (12)$$

where

$$\begin{aligned} \alpha_1 &= \tan A_1' [\tan Q' + \rho_c \tan (P_1' - Q')] \\ \gamma_1 &= \rho_c \tan (P_1' - Q') \tan Q' \\ \beta_1 &= \alpha_1 / (\sin A_1') + \\ & \quad [\tan A_1' - \alpha_1 \rho_c \tan (P_1' - Q') / \gamma_1] / \cos^2 Q' . \end{aligned} \quad (13)$$

Similar formulas apply to the other set ( $P_2$ ,  $A_2$ , and  $Q$ ) so

$$\rho = \frac{\alpha_1 + \beta_1 \delta}{\gamma_1} = \frac{\alpha_2 + \beta_2 \delta}{\gamma_2} . \quad (14)$$

Solving for the angle of tilt gives

$$\delta = \frac{\alpha_2 \gamma_1 - \alpha_1 \gamma_2}{\beta_1 \gamma_2 - \beta_2 \gamma_1} . \quad (15)$$

When  $\delta$  is calculated, the azimuths are corrected by eq 9 and  $\rho$  is calculated by eq 3.



### 3.4. Calculation of the Thickness of a Film from $\Delta$ and $\psi$

This calculation has been previously described [4], but since the final formulas were not given, they are summarized here.

The total reflection coefficients  $R^P$  and  $R^S$  for light polarized parallel and perpendicular to the plane of incidence are given by

$$R^P = \frac{r_{12}^P + r_{23}^P Y}{1 + r_{12}^P r_{23}^P Y}$$

$$R^n = \frac{r_{12}^n + r_{23}^n Y}{1 + r_{12}^n r_{23}^n Y} \quad (16)$$

where  $r_{12}^P$ ,  $r_{23}^P$ ,  $r_{12}^n$ , and  $r_{23}^n$  are the reflection coefficients between medium and film (indices 1 and 2) and between the film and substrate (indices 2 and 3).

$$Y = \exp[-4\pi i n_2 \cos\varphi_2 d_2/\lambda] \quad (17)$$

where  $n_2$  and  $d_2$  are the index of refraction and thickness of the film and  $\varphi_2$  is the angle for light in the film given by

$$\cos\varphi_2 = [1 - (n_1 \sin\varphi_1/n_2)^2]^{1/2}. \quad (18)$$

The ellipsometer readings determine

$$\rho = \tan\psi \exp(i\Delta) = R^P/R^S. \quad (19)$$

From eqs 16 and 19,

$$EY^2 + BY + C = 0, \quad (20)$$

where

$$E = \rho r_{21}^P r_{32}^P r_{32}^n - r_n^{21} r_{32}^P r_{32}^n$$

$$B = \rho(r_{32}^n + r_{21}^p r_{21}^n r_{32}^p) - r_p^{32} - r_{21}^p r_{21}^n r_{32}^n$$

$$C = \rho r_{21}^n - r_{21}^p \quad . \quad (21)$$

The two solutions of eq 20

$$Y_1 = [-B + (B^2 - 4EC)^{\frac{1}{2}}] / 2E \quad (22)$$

$$Y_2 = [-B - (B^2 - 4EC)^{\frac{1}{2}}] / 2E \quad (23)$$

are calculated. Then, from each solution a value for the film thickness  $d_2$  is calculated. These values, called D2C1 and D2C2 are calculated by subroutine CALDX.

These values are complex numbers. Since the film thickness is a real number, the imaginary part is due to error in either the ellipsometer readings or the values of the refractive indices or in the angle of incidence used for the calculation, so must be small. Therefore, the value of D2C1 or D2C2 with the smallest imaginary part is taken as the correct solution. The real part is taken as the film thickness while the imaginary part is taken as a measure of error.

### 3.5. Calculation of Both the Refractive Index and Thickness of a Film From Values of $\Delta$ and $\psi$

The preceding section described the calculation of the thickness of a film for a given value of the refractive index of a film. Two complex numbers, D2C1 and D2C2, were obtained for the film thickness. The real parts of the numbers were taken as the film thickness and the corresponding imaginary parts as measures of error.

The subroutine SØLN2 determines the refractive index of the film that will minimize the absolute error of the error term.

For simplicity, we consider that the index of the film is real, i.e.,  $\kappa=0$ . The calculations may also be performed for a given value of  $\kappa$ .

The method requires limits,  $n_2'$  and  $n_2''$ , for the refractive index  $n_2$  of the film, such that  $n_2' < n_2''$ . First, the complex film thickness D2C1 is computed with  $n_2'$  and  $n_2''$  used for the index. Since the error term, the imaginary part of D2C1, is zero for the correct value of  $n_2$ , it is expected to change sign as  $n_2$  is varied from  $n_2'$  to  $n_2''$ . Therefore, if the error terms for  $n_2'$  and  $n_2''$  have the same sign, it is assumed that no solution for  $n_2$  exists using D2C1 for the film thickness. See figure 11a.

If the error terms have different signs for indices  $n_2'$  and  $n_2''$ , the error term is evaluated for the intermediate index  $n_2''' = (n_2' + n_2'')/2$ . Then the interval containing the index  $n_2$  is narrowed by consideration of signs of the error terms. For example, suppose that the signs of the error terms for the indices  $n_2'$ ,  $n_2'''$ ,  $n_2''$  are -, -, +, respectively. Then the error term changes sign from  $n_2'''$  to  $n_2''$  so the solution for  $n_2$  for which the error term is zero must lie in this range. That is  $n_2''' < n_2 < n_2''$ .

The value of  $n_2'''$  is then tested to determine if it is sufficiently close to the solution for  $n_2$ . This is done by computing values of  $\Delta$  and  $\psi$  using the real part of D2D1 for the film thickness. Of course, use of the complex value of D2C1 for the film thickness would give the experimental values of  $\Delta$  and  $\psi$ , but dropping the imaginary part will change the computed values of  $\Delta$  and  $\psi$ . The value of  $n_2'''$  is then judged to be sufficiently close to the solution for  $n_2$  if the computed values of  $\Delta$  and  $\psi$  are both within  $0.005^\circ$  of the experimental values. If the differences between the computed and experimental values of  $\Delta$  and  $\psi$  are larger than  $0.005^\circ$ , the range is further reduced until they agree to within  $.005^\circ$ . (This value of  $0.005^\circ$  can be changed by the ELDP instruction.) The process is then repeated using D2C2.

Note that the values given by the ELDP instruction determine the closeness of the search for the refractive index  $n_2$  of the film. They should be less than the experimental errors of  $\Delta$  and  $\psi$ , but if they are too small, the computation time will be excessive.

Figure 11a shows a possible relationship of the error term to assumed values of the film index. For the limiting values of  $n_2'$  and  $n_2''$  of the index, the signs of the error terms are different (- and +) so the computer will search for a solution by computing the error term for the intermediate index  $n_2'''$ . The signs of the error terms corresponding to  $n_2'$ ,  $n_2'''$ , and  $n_2''$  are -, -, and +, respectively. The solution is then correctly determined to lie between  $n_2'''$  and  $n_2''$  and this range will be subdivided. The procedure is seen to converge to the solution  $n_2$ .

Cases in which the procedure fails are shown in figures 11b to 11d. In figure 11b the error terms are of the same sign (positive) for both  $n_2'$  and  $n_2''$  so the computer assumes that no solution exists. However, there is a solution,  $n_2$ , outside the assumed range. In this case, too narrow a range for  $n_2$  was used.

In figure 11c the error terms corresponding to the limits  $n_2'$  and  $n_2''$  are also of the same sign (positive) so no solution will be found although two solutions between  $n_2'$  and  $n_2''$  exist. In this case, the assumed range was too broad. If the range has been subdivided and both sections searched for a solution, both solutions for  $n_2$  would have been obtained.

In figure 11d the error terms for  $n_2'$  and  $n_2''$  have different signs so the computer will search for a solution by first computing the error term for index  $n_2'''$ . The signs of the error corresponding to  $n_2'$ ,  $n_2'''$ , and  $n_2''$  are +, -, -, so the computer will continue the search in the interval  $n_2'$  to  $n_2'''$  and converge to the solution. However, the two solutions between  $n_2'''$  and  $n_2''$  will be missed. Again, the range of the index must be subdivided to obtain all the solutions.



### 3.6. Confidence Limits for the Refractive Index and Thickness of a Film

The preceding section described the calculation of the refractive index and thickness of a film from measured values of  $\Delta$  and  $\psi$  as performed by the instruction CND. Instruction CNDC performs the same calculations and, in addition, calculates the uncertainty in the refractive index and thickness due to uncertainty in the values of  $\Delta$  and  $\psi$ .

Let the measured values of  $\Delta$  and  $\psi$  be  $\Delta_0$  and  $\psi_0$  and let their 95 percent confidence limits be  $\Delta_0 - \delta\Delta$  to  $\Delta_0 + \delta\Delta$  and  $\psi_0 - \delta\psi$  to  $\psi_0 + \delta\psi$ . That is, the true value of  $\Delta$  lies between  $\Delta_0 - \delta\Delta$  and  $\Delta_0 + \delta\Delta$  with 95 percent probability, and similarly for  $\psi$ . ( $\delta\Delta$  and  $\delta\psi$  equal 1.96 times the standard deviations of  $\Delta$  and  $\psi$  when based on a large number of degrees of freedom.) Then both  $\Delta$  and  $\psi$  will lie within the joint confidence ellipse (also called contour ellipse)  $(\Delta - \Delta_0)^2 / (\delta\Delta)^2 + (\psi - \psi_0)^2 / (\delta\psi)^2 = 1.560$  with 95 percent probability\* [11, 12]. An example is shown in figure 5. For each value of  $\Delta$  and  $\psi$  on the ellipse, values of  $n_2$  and  $d_2$ , the refractive index and thickness of the film, may be calculated. Plotting these values of  $n_2$  versus  $d_2$ , a curve, approximately an ellipse, is obtained as illustrated in figure 6. This curve is the 95 percent joint confidence curve for  $n_2$  and  $d_2$ ; i.e., the true values of  $n_2$  and  $d_2$  lie within this curve with 95 percent probability.

The instruction CNDC determines eight points of the joint confidence curve for  $n_2$  and  $d_2$ . The maximum and minimum values of  $n_2$  and  $d_2$  are also printed as their individual confidence limits. The instruction CNDE performs the same calculations as CNDC but prints only the individual confidence limits of  $n_2$  and  $d_2$ .

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\*The equation of the joint confidence ellipse is generally written in terms of standard deviations. For convenience, we have expressed it in terms of 95 percent confidence limits.

The confidence limits for  $\Delta$  and  $\psi$ ,  $\delta\Delta$  and  $\delta\psi$ , are given by an EDP instruction before the CNDC or CNDE instruction. If an EDP instruction is not given, the value  $0.015^\circ$  is used for both  $\delta\Delta$  and  $\delta\psi$ .

### 3.7. Volume Fractions and Total Amount of Material for a Film Composed of a Mixture of Two Materials

Consider a film that is a mixture of the immersion medium of refractive index  $n_1$  and density  $\rho_1$  and a material of index  $n_p$  and density  $\rho_p$ . Let the refractive index of the film that has been calculated be  $n_f$ . We desire to compute the weight fraction,  $f$ , of the material in the film.

The specific refraction,  $S_f$ , of the film is additive in the specific refractions of the medium,  $S_1$ , and the material,  $S_p$ . Thus

$$S_f/\rho_f = f S_p/\rho_p + (1-f) S_1/\rho_1, \quad (24)$$

where  $\rho_f$  is density of the film and  $S_f = (n_f^2 - 1)/(n_f^2 + 2)$  and similarly for  $S_1$  and  $S_p$ . To determine the density of the film, we have the volume of a unit weight of the film as  $f/\rho_p + (1-f)/\rho_1$  assuming additivity of the partial volumes of the components of the film. Therefore, the density of the film is

$$\rho_f = 1/[f/\rho_p + (1-f)/\rho_1]. \quad (25)$$

Substituting in the previous equation and solving for  $f$  gives

$$f = \frac{\rho_p}{\rho_p + (S_f - S_p)\rho_1 / (S_1 - S_f)}. \quad (26)$$

The amount of material per unit area of film is  $\rho_f d_2 f$  where  $d_2$  is the thickness of the film. If the densities are in  $\text{g/cm}^3$  and the film thickness in  $\text{\AA}$ , the amount of material per unit area of film in  $\text{mg/cm}^2$  is given by  $10^{-5} \rho_f d f$ .

### 3.8. Computation of Ellipsometer Readings From $\Delta$ and $\psi$

Substituting eqs 1 and 2 in eq 3 and rearranging gives

$$\frac{\tan A}{\tan \psi} = \frac{(\cos \Delta + i \sin \Delta) [T_c \tan Q \tan(P-Q)(\cos \Delta_c - i \sin \Delta_c) - 1]}{\tan Q + T_c \tan(P-Q)(\cos \Delta_c - i \sin \Delta_c)} \quad (27)$$

This expression is reduced to the form of a real and imaginary term. Then, the imaginary term must be zero since  $\tan A / \tan \psi$  is real. Solving gives

$$\tan(P-Q) = (-R \pm \sqrt{R^2 + 1}) / T_c, \quad (28)$$

where

$$R = \frac{\tan Q \sin(\Delta - \Delta_c) - \sin(\Delta + \Delta_c) / \tan Q}{2 \sin \Delta} \quad (29)$$

or

$$P = \arctan[(-R \pm \sqrt{R^2 + 1}) / T_c] + Q. \quad (30)$$

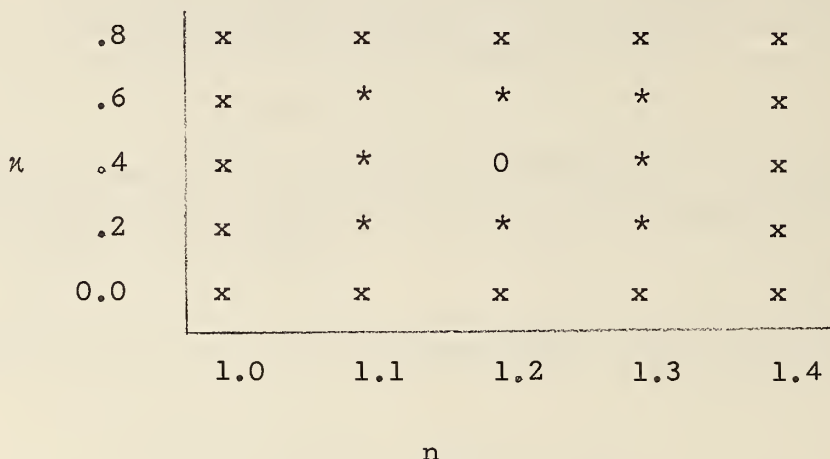
Two values of P are thus calculated. A value of A may be calculated by eq 27 for each value of P.

### 3.9. Computation of $n$ and $\kappa$ of a Film of Given Thickness

This computation is best described by considering the instructions

NS	2.5					
FT	50.					
NF	1.1	0.1	1.3	0.2	0.2	0.2
CNK	90.5	32.				

The computer searches for a value of  $n$  between 1.1 and 1.3 and a value of  $\kappa$  between 0.2 and 0.6 for a film of 50 Å thickness that will give values of  $\Delta$  and  $\psi$  near  $90.5^\circ$  and  $32^\circ$ . First, the computer increases the range of  $n$  and  $\kappa$  by their increments. That is, the range of  $n$  becomes 1.1-0.1 to 1.3+.1 and the range of  $\kappa$  becomes 0.2-0.2 to 0.6+0.2. This is graphically illustrated below.



Increasing the ranges of  $n$  and  $\kappa$  prevents solutions near the boundary of the range being missed in the searching procedure.

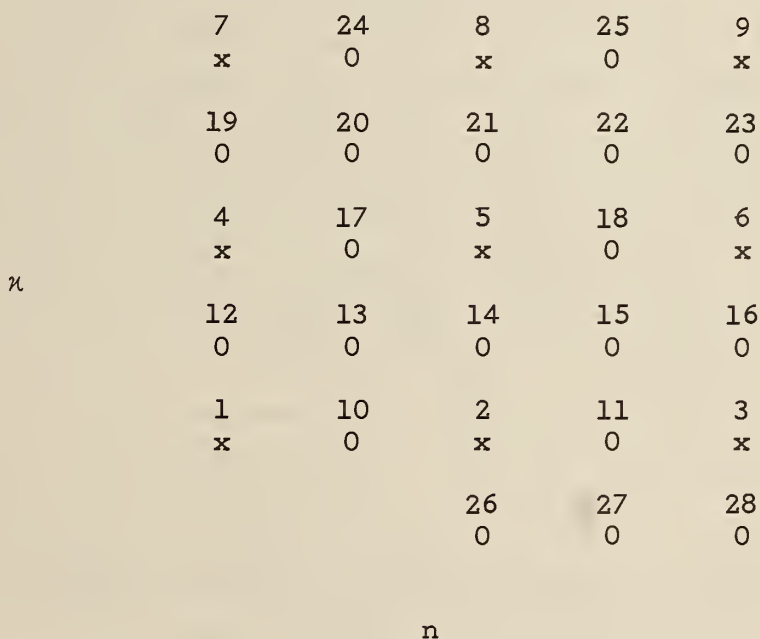
For every pair of values of  $n$  and  $\kappa$  in this figure an error term  $|\rho_c - \rho_e|$  is computed. In this error term,  $\rho_c$  is the value of  $\rho$  computed for the value of  $n$ ,  $\kappa$  and thickness of the film, and  $\rho_e$  is the value of  $\rho$  corresponding to the values of  $\Delta$  and  $\psi$  (eq 1) given with the CNK instruction. This error term is zero only when the values of  $n$  and  $\kappa$  are a solution, and is small when  $n$  and  $\kappa$  are near a solution. Therefore, the computation consists of searching for values of  $n$  and  $\kappa$  that minimize the error time.

This is accomplished by comparing each error term with the error term at surrounding points. If the error term is less than that at the surrounding points, a minimum is assumed to occur near the value of  $n$  and  $\kappa$  for the error term. For example, in the above figure, if the error term for  $n=1.2$  and  $\kappa=0.4$  (represented by 0) is



less than the surrounding error terms represented by \*, a minimum of the error term is tentatively assumed to occur in the range of  $n=1.1$  to  $1.3$  and  $\kappa=0.2$  to  $0.6$ . All interior points of the grid of  $n$  and  $\kappa$  values are thus tested.

The next step is to search the range of  $n$  and  $\kappa$  to locate the minimum. This procedure is illustrated by the following figure.



This figure represents the ranges of  $n$  and  $\kappa$  for which a minimum is found to occur. That is, the error terms at points 1 to 9,  $F_1$  to  $F_9$  (represented by x on the figure) have been calculated and the error term to point 5,  $F_5$ , has been found to be less than  $F_1$ ,  $F_2$ ,  $F_3$ ,  $F_4$ ,  $F_6$ ,  $F_7$ ,  $F_8$ , and  $F_9$ . The procedure is to calculate the error term at point 13,  $F_{13}$ . If it is greater than  $F_5$ ,  $F_{14}$  is calculated. If  $F_{14}$  is also greater than  $F_5$ ,  $F_{15}$  is calculated, and so forth. If  $F_{13}$ ,  $F_{14}$ ,  $F_{15}$ ,  $F_{18}$ ,  $F_{22}$ ,  $F_{21}$ ,  $F_{20}$ , and  $F_{17}$  are all greater than  $F_5$ , they define a new reduced range for the minimum and the process is repeated.

Consider the case that one of the terms, say  $F_{15}$ , is less than  $F_5$ . Then  $F_{15}$  is also less than  $F_2$ ,  $F_3$ ,  $F_6$ , and  $F_{14}$  since these terms are greater than  $F_5$ . Terms  $F_{11}$ ,  $F_{16}$ , and  $F_{18}$  are then calculated. If these terms are all greater than  $F_{15}$ , a new reduced range centered around  $F_{15}$  is found and the process is repeated.

Next, consider the case that one of these terms, say  $F_{11}$ , is less than  $F_{15}$ . In this case terms  $F_{26}$ ,  $F_{27}$ , and  $F_{28}$  are computed. If these terms are all greater than  $F_{11}$ , a range centered around  $F_{11}$  is found. However, if one of these terms, say  $F_{26}$ , is less than  $F_{11}$ , another process to follow the minimum is used. All eight terms surrounding  $F_{26}$  are calculated and if any of them is less than  $F_{26}$ , its eight surrounding terms are calculated and compared with its value. This secondary process is repeated five times. If an error term less than its eight surrounding terms is obtained, the process of reducing the range continues. If not, the process is considered to fail and a diagnostic message printed.

The process of reducing the range is repeated ten times, thereby reducing the original range by a factor of about 2000. These calculations are performed by the subroutine MIN2V and the error terms are calculated by the function FUNC.

Oldham [14] has programed and tested another method for determining the optical properties of adsorbing films of given thickness from ellipsometer readings. His method is a generalization for complex variables of Newton's method of finding roots of a function. His method probably finds solutions with less calculation than the method used in this program. However, it is more likely to fail in finding solutions and does not ordinarily give multiple solutions as does the method used in this program.

#### 4. The Fortran Program

This computer program was originally written in Fortran V for use with the Univac 1108 computer. Because some of the features of this Fortran compiler do not apply to other Fortran compilers, the program in Fortran IV is given in Section 4.1. The data input preceding is identical for both programs except for the instructions discussed in Section 2.12. With the Fortran IV program the first card of the data and the card following the PAGE and RESET instructions must be a comment card, and no other comment cards may be used in the program. Also, comments may not be placed on the PAGE and RESET instruction cards. These restrictions are required because the instruction of the form, READ (0,i) List, in Fortran V is not generally available in Fortran IV.

The Fortran IV program used logical unit 5 for input and logical unit 6 for output. These logical unit numbers may have to be changed for some computers.

For both versions of the program, complex and real values are combined in arithmetic statements with the result being complex.

The Fortran V version of the program and both versions on cards are available from the author.

4.1 FORTRAN IV PROGRAM

```

C      CALCULATION FOR ELLIPSOMETER
C      FOR IFILM, THE NUMBER OF FILMS ADD. RESET IS NECESSARY TO ERASE FILMS
C      CHANGED TO USE KAPPA INSTEAD OF IMAGINARY PART OF REFRACTIVE INDEX
      DIMENSION IDT(14),FNSI(2),DFNS(2),FNSE(2),FNSX(2),TN(8),TD(8)
      DIMENSION INST(31)
      COMMON FN1,S1,C1,N,FNX(900),D(900),FN2,CRP,CRN,CRP32,CRN32,WL,
1  RP21,RN21,DEL,PSI,C2,C3,FN2I(2),DFN2(2),FN2E(2),FN2X(2),T1,T2,T3,
2  T4,D2,DELDX,PSIDX, ELDEL,ELPSI,DENP,FNP,DEN1,MX,K,IS
      COMPLEX C2,C3,C1,CIP1,CN,CNM1,CRN,CRN21,CRN32,CRP,CRP21,CRP32
      COMPLEX FN2,FNX,FNS, RHO,RN,RN21, RP,RP21, RC,SRC
      COMPLEX T1,T2,T3,T4,RHOC,RH01,RH02,CAT,ALP1,ALP2,BET1,BET2
      COMPLEX GAM1,GAM2,CAT
C      INSTRUCTIONS TO BE COMPARED WITH INSTRUCTIONS GIVEN WITH
C      DATA
C      M=      1      2      3      4      5      6
C      DATA INST/6HPAGE ,6HNM ,6HNF ,6HNS ,6HAI ,6HWL ,
C      7      8      9      10      11      12      13
C      1 6HWP ,6HREF ,6HEDP ,6HELDP ,6HRESET ,6HFILM ,6HMIXED ,
C      14      15      16      17      18      19      20
C      2 6HCTABLE,6HCD ,6HCND ,6HCNDE ,6HCNDC ,6HCNS ,6HCWP ,
C      21      22      23      24      25      26      27
C      3 6HCDN ,6HCDNE ,6HCDNC ,6HAT ,6HCAT ,6HCATA ,6HIFILM ,
C      28      29      30 31
C      4 6HALINE ,6HSTOP ,2HFT,3HCNK/
C      SRC IS SMALL REFLECTION COEFFICIENT (WITHOUT CONSIDERING
C      UNDERLYING LAYERS)
      SRC(A,B)=(A-B)/(A+B)
C      SIN,COS,ATAN,TAN FOR ANGLES IN DEGREES
      SIND (X)=SIN(X/57.29578)
      COSD (X)=COS(X/57.29578)
      ATAND (X)=ATAN(X)*57.29578
      TAND(X)=SIND(X)/COSD(X)
C      S IS USED FOR CALCULATING SPECIFIC REFRACTION
      S(XN)=(XN*XN-1.)/(XN*XN+2.)
C      GIVE STANDARD VALUES TO VARIABLES
10 FN1I=1.
   DFN1=0.
   FN1E=0.
   AT=0.
   ALP=0.
   ALA=0.
   ALQ=0.
   FN2I(1)=1.
   FN2I(2)=0.
   DFN2(1)=0.
   DFN2(2)=0.
   FN2E(1)=0.
   FN2E(2)=0.
   FNSI(1)=1.
   FNSI(2)=0.
   DFNS(1)=0.
   DFNS(2)=0.
   FNSE(1)=0.
   FNSE(2)=0.
   AII=70.
   AIE=0.
   WLI=5461.

```



```

DWL=0.
WLE=0.
RHOC=(0.,-1.)
TC=1.
DELC=90.
DEN1=1.
DENP=1.
FNP=1.5
N=2
ELDEL=.002
ELPSI=.002
D2I=0.
DD2=0.
D2F=0.
FN=1.
EDEL=.015
EPSI=.015
C      READ AND PRINT TITLE CARD
12 READ(5,15) IDT
15 FORMAT(13A6,A2)
   WRITE(6,17) IDT
17 FORMAT(1H1,14A6)
C      READ AND PRINT CARD OF DATA
20 READ(5,25) L,Z1,Z2,Z3,Z4,Z5,Z6
25 FORMAT(A6,3X,6F10.0)
   WRITE(6,27) L,Z1,Z2,Z3,Z4,Z5,Z6
27 FORMAT(1H ,A6,3X,6F15.5)
C      COMPARE L WITH INSTRUCTIONS TO FIND M.
   DO 30 M=1,31
30   IF(L.EQ.INST(M)) GO TO 35
   GO TO 20
C      M= 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16
35   GO TO(12,50,70,80,90,100,110,120,130,140,10,150,160,305,170,170,
C      17 18 19 20 21 22 23 24 25 26 27 28 29 30 31
   1 170,170,170,730,170,170,170,250,750,750,270,260,810,305,170),M
C      INSTRUCTION NM, REFRACTIVE INDEX OF MEDIUM
50   FN1I=Z1
   DFN1=Z2
   FN1E=1.000001*Z3
   GO TO 20
C      INSTRUCTION NF, REFRACTIVE INDEX OF TOP FILM
70   FN2I(1)=Z1
   DFN2(1)=Z2
   FN2E(1)=1.000001*Z3
   FN2I(2)=Z4
   DFN2(2)=Z5
   FN2E(2)=1.000001*Z6
C      IF DFN2(1) IS LEFT BLANK ON DATA CARD, SUBSTITUTE A VALUE OF
C      DFN2(1) SO THAT ONLY ONE CALCULATION WILL BE PERFORMED.
   IF(ABS(DFN2(1)).EQ.0.) DFN2(1)=1.000002*ABS(FN2E(1)-FN2I(1))
C      INSTRUCTION NS, REFRACTIVE INDEX OF SUBSTRATE
80   FNSI(1)=Z1
   DFNS(1)=Z2
   FNSE(1)=1.000001*Z3
   FNSI(2)=Z4
   DFNS(2)=Z5
   FNSE(2)=1.000001*Z6
   GO TO 20
C      INSTRUCTION AI, ANGLE OF INCIDENCE
90   AII=Z1
   DAI=Z2
   AIE=1.000001*Z3

```

```

GO TO 20
C   INSTRUCTION WL, WAVE LENGTH OF LIGHT
100 WLI=Z1
    DWL=Z2
    WLE=1.000001*Z3
    GO TO 20
C   INSTRUCTION WP, CONSTANTS OF WAVE PLATE
110 TC=Z1
    DELC=Z2
    RHOC=TC*CEXP((0.,-1.)*DELC/57.29578)
    GO TO 20
C   INSTRUCTION NREF, NUMBER OF REFLECTIONS OF THE LIGHT
120 FN=Z1
    GO TO 20
C   INSTRUCTION EDP, CONFIDENCE FIMITS FOR DELTA AND PSI
130 EDEL=Z1
    EPSI=Z2
    GO TO 20
C   INSTRUCTION ELDP, ERROR LIMITS FOR DELTA AND PSI
140 ELDEL=Z1
    ELPSI=Z2
    GO TO 20
C   INSTRUCTION FILM ,NUMBER, THICKNESS AND REFRACTIVE INDEX OF FILM
150 I=1.000001*Z1+1
    D(I)=Z2
    FNX(I)=CMPLX(Z3,-Z3*ABS(Z4))
    N=MAX0(N,I)
    GO TO 20
C   INSTRUCTION MIXED, DATA FOR MIXED FILMS
160 DEN1=Z1
    DENP=Z2
    FNP=Z3
    GO TO 20
C   VALUES OF DELTA AND PSI OR OF P,A,AND Q HAVE BEEN GIVEN
C   USE PREVIOUS VALUES OF DEL AND PSI IF NO DATA IS GIVEN,Z1=Z2=0
C   IF FIRST VALUE(Z1) =0,USE PREVIOUSLY GIVEN VALUES OF
C   DELTA AND PSI
170 IF(ABS(Z1).EQ.0.) GO TO 310
    IF(ABS(Z5).EQ.0.) GO TO 180
C   Z5 NOT =0, SO P1,A1,P2,A2,Q ARE GIVEN
C   COMPUTE TWO VALUES OF RHO
    Z1=Z1+AT+ALP
    Z2=Z2+AT+ALA
    Z3=Z3+AT+ALP
    Z4=Z4+AT+ALA
    Z5=Z5+AT+ALQ
    WRITE(6,27) L,Z1,Z2,Z3,Z4,Z5
174 RH01=TAND(Z2)*(TAND(Z5)+TAND(Z1-Z5)*RHOC)/(TAND(Z1-Z5)*TAND(Z5)*
1   RHOC-1.)
    RH02=TAND(Z4)*(TAND(Z5)+TAND(Z3-Z5)*RHOC)/(TAND(Z3-Z5)*TAND(Z5)*
1   RHOC-1.)
C   AVERAGE VALUES OF RHO,COMPUTE VALUES OF DELTA AND PSI
    RH0=(RH01+RH02)/2.
    DEL1=ATAN2(AIMAG(RH01),REAL(RH01))*57.29578
    PSI1=ATAND(CABS(RH01))
    DEL2=ATAN2(AIMAG(RH02),REAL(RH02))*57.29578
    PSI2=ATAND(CABS(RH02))
    WRITE(6,175) DEL1,PSI1,DEL2,PSI2
175 FORMAT(6H DEL1=,F12.6,6H PSI1=,F12.6,6H DEL2=,F12.6,
1   6H PSI2=,F12.6)
    IF(FN.EQ.1.) GO TO 210
    GO TO 200

```

```

C           IF Z3=0, DELTA AND PSI ARE GIVEN, OTHERWISE P,A,Q ARE GIVEN
180 IF(ABS(Z3).EQ.0.) GO TO 190
      Z1=Z1+AT+ALP
      Z2=Z2+AT+ALA
      Z3=Z3+AT+ALQ
      WRITE(6,27) L,Z1,Z2,Z3
185 RHO=TAND(Z2)*(TAND(Z3)+TAND(Z1-Z3)*RHOC)/(TAND(Z1-Z3)*TAND(Z3)*
      1 RHOC-1.)
      IF(FN.EQ.1.) GO TO 210
      GO TO 200
190 DEL=Z1
      PSI=Z2
      RHO=TAND(PSI)*CEXP((0.,1.)*DEL/57.29578)
      IF(FN.EQ.1.) GO TO 310
C           CORRECT FOR NUMBER OF REFLECTIONS IF FN NOT =1
200 RHO=CEXP(1./FN*CLOG(RHO))
210 DEL=ATAN2(AIMAG(RHO),REAL(RHO))*57.29578
      PSI=ATAND(CABS(RHO))
      IF(M.EQ.25 .OR. M.EQ.26) GO TO 755
215 WRITE(6,220) DEL,PSI
220 FORMAT(6H DEL=,F13.6,5H PSI=,F13.6)
      GO TO 310
C           INSTRUCTION AT, ANGLE OF TILT OF SAMPLE
250 AT=Z1
      GO TO 20
C           INSTRUCTION ALINE, ALINEMENT CORRECTIONS
260 ALP=Z1
      ALA=Z2
      ALQ=Z3
      GO TO 20
C           INSTRUCTION IFILM, CALCULATES THICKNESSES AND REFRACTIVE
C           INDICES OF A SERIES OF FILMS
270 XNF=Z1
      TH=Z2
C           REMOVE ALL PREVIOUSLY DESIGNATED FILMS.
C           WITHOUT NEXT CARD, FILMS WILL BE PLACED BETWEEN PREVIOUSLY
C           DESIGNATED FILMS AND SUBSTRATE
      N=2
C           DN AND DK ARE INCREMENTS OF REFRACTIVE INDEX AND K
      DN=(Z5-Z3)/XNF
      DK=(Z6-Z4)/XNF
C           COMPUTE INDEX AND K (KAPPA) OF TOP FILM
      Z3=Z3+DN/2.
      Z4=Z4+DK/2.
C           INDEX OF TOP FILM IS N1, INDEX OF BOTTOM FILM IS N
      N1=N+1
      NF=1.000001*XNF
      N=N+NF
      DO 280 I=N1,N
      D(I)=TH/NF
      FN(I)=CMPLX(Z3,-Z3*Z4)
      Z3=Z3+DN
280 Z4=Z4+DK
      GO TO 20
C           THICKNESS OF TOP FILM AND ,OPTIONALLLY, SETTING OF WAVE PLATE
305 D21=Z1
      DD2=Z2
      D2E=1.000001*Z3
      Q=Z4
      IF(M.EQ.30) GO TO 20
C           SET INITIAL VALUES
310 FN1=FN1I

```

```

311 AI=AI
312 S1=SIND(AI)
    C1=COSD(AI)
    IF(M.EQ.19) GO TO 710
315 WL=WLI
    WRITE (6,316) FN1,AI,WL,TC,DELC
316 FORMAT(17H0INDEX OF MEDIUM=,F10.5,21H ANGLE OF INCIDENCE=,F10.3,
    1 14H WAVE LENGTH=,F10.2,5H TC=,F10.5,7H DELC=,F10.3)
    IF(M.EQ.14) GO TO 320
    IF(M.EQ.31) GO TO 318
C      PRINT TABLE HEADINGS EXCEPT FOR CTABLE OR CNK
    WRITE(6,317)
317 FORMAT(123H0 THICK NF REAL KAPPA ADSORPTION D DEL D P
    1SI ERROR NF-NM NS-NF WT FRACTION NS REAL KAPPA
    2 K)
    GO TO 320
C      PRINT HEADINGS FOR INSTRUCTION CNK
318 PRINT 319
319 FORMAT(1H0,8X,2HNF,15X,5HKAPPA,9X,4HD NF,11X,7HD KAPPA,9X,
    1 5HERROR,3X,7HD DELTA,5X,5HD PSI,10X,5HTHICK)
320 NP1=N+1
C      SET VALUES FOR REFRACTIVE INDEX OF SUBSTRATE
325 FNSX(1)=FNSI(1)
326 FNSX(2)=FNSI(2)
327 FNX(NP1)=CMLPX(FNSX(1),-FNSX(2)*FNSX(1))
C      COMPUTE REFLECTION COEF BETWEEN LAYERS 3 AND 4
    IF(N.EQ.2) GO TO 335
    X=SIND(AI)*FN1
    CN=CSQRT(1.-(X/FNX(N+1))**2)
    CNM1=CSQRT(1.-(X/FNX(N))**2)
    CRP=SRC(FNX(N+1)*CNM1,FNX(N)*CN)
    CRN=SRC(FNX(N)*CNM1,FNX(N+1)*CN)
    IF(N.EQ.3) GO TO 335
    NX=N-3
    I=N-1
    DO 330 J=1,NX
        CIP1=CSQRT(1.-(X/FNX(I+1))**2)
        CI= CSQRT(1.-(X/FNX(I)) **2)
        RP=SRC(FNX(I+1)*CI,FNX(I)*CIP1)
        RN=SRC(FNX(I)*CI,FNX(I+1)*CIP1)
        T1=FNX(I+1)*CIP1*D(I+1)/WL
        CRP=RC(RP,CRP,T1)
        CRN=RC(RN,CRN,T1)
330 I=I-1
335 IF(M.EQ.31) GO TO 850
340 FN2X(2)=FN2I(2)
342 FN2X(1)=FN2I(1)
343 FN2=CMLPX(FN2X(1),-FN2X(2)*FN2X(1))
C      CALCULATE REFLECTION COEF BETWEEN LAYERS 2 AND 3
    CALL CRC
    IF(M.EQ.14) GO TO 350
    K=1
C      EXCEPT FOR CTABLE,CALCULATE VALUES,T1 AND T2, OF FILM
C      THICKNESS
    CALL CALDX (T1,T2)
    IF(M.EQ.15) GO TO 455
C      EXCEPT FOR CTABLE OR CD,CALCULATE COMPLEX VALUES,T3 AND
C      T4 OF FILM THICKNESS FOR UPPER VALUE OF FILM
C      REFRACTIVE INDEX
    FN2=CMLPX(FN2X(1)+DFN2(1),-FN2X(2)*(FN2X(1)+DFN2(1)))
    CALL CRC
    CALL CALDX(T3,T4)

```



```

C   IS=1 FOR NO SOLUTION FOUND   IS=2 FOR SOLUTION FOUND
      IS=1
      IF(( AIMAG(T1).GT.0..AND.AIMAG(T3).LT.0.).OR.(AIMAG(T1).LT.0..AND.
1     AIMAG(T3).GT.0.)) GO TO 485
C   NO SOLUTION FOR N2 FOR FIRST SOLUTION OF QUADRATIC
345 IF((AIMAG(T2).GT.0..AND.AIMAG(T4).LT.0.).OR.(AIMAG(T2).LT.0..AND.
1     AIMAG(T4).GT.0.)) GO TO 487
C   NO SOLUTION FOR N2 FOR SECOND SOLUTION OF QUADRATIC
347 IF (IS.EQ.2) GO TO 670
C   NO SOLUTION FOUND, TRY OTHER QUADRANTS FOR SQRT IN CALDX
      K=3
      FN2=CMPLX(FN2X(1),-FN2X(2)*FN2X(1))
      CALL CRC
      CALL CALDX (T1,T2)
      FN2=CMPLX(FN2X(1)+DFN2(1),-FN2X(2)*(FN2X(1)+DFN2(1)))
      CALL CRC
      CALL CALDX(T3,T4)
      IF(( AIMAG(T1).GT.0..AND.AIMAG(T3).LT.0.).OR.(AIMAG(T1).LT.0..AND.
1     AIMAG(T3).GT.0.)) GO TO 490
348 IF((AIMAG(T2).GT.0..AND.AIMAG(T4).LT.0.).OR.(AIMAG(T2).LT.0..AND.
1     AIMAG(T4).GT.0.)) GO TO 489
      GO TO 670
C   TABLES OF DEL AND PSI FOR CTABLE
350 WRITE(6,360)
360 FORMAT(1H0,3X,5HTHICK,4X,3HDEL,5X,3HPSI,4X,14HRF.CF.PARALLEL,6X,
1     12HRF.CF.NORMAL,4X,2HNF,4X,5HKAPPA,2X,2HNS,5X,5HKAPPA,4H,
2     2HP1,5X,2HA1,5X,2HP2,5X,2HA2)
390 D2=D2I
400 CRP21=RC(RP21,CRP32,FN2*C2*D2/WL)
      CRN21=RC(RN21,CRN32,FN2*C2*D2/WL)
      RHO=CRP21/CRN21
      IF(FN.NE.1.) RHO=CEXP(1./FN*CLOG(RHO))
      DEL=ATAN2(AIMAG(RHO),REAL(RHO))*57.29578
      IF(REAL(RHO).LT.0. .AND. ABS(AIMAG(RHO)).LT. 1.0E-6) DEL=180.
      PSI=ATAND(CABS(RHO))
      XM1=CABS(CRP21)
      THETA1=ATAN2(AIMAG(CRP21),REAL(CRP21))*57.29578
      IF(REAL(CRP21).LT.0. .AND. ABS(AIMAG(CRP21)).LT.1.0E-6) THETA1=180.
      XM2=CABS(CRN21)
      THETA2=ATAN2(AIMAG(CRN21),REAL(CRN21))*57.29578
      IF(REAL(CRN21).LT.0. .AND. ABS(AIMAG(CRN21)).LT.1.0E-6) THETA2=180.
      FN2R=REAL(FN2)
      FNXR=REAL(FNX(N+1))
      FK2=-AIMAG(FN2)/REAL(FN2)
      FKX=-AIMAG(FNX(N+1))/REAL(FNX(N+1))
      IF(ABS(Q).NE.0.) GO TO 420
      WRITE(6,410) D2,DEL,PSI,XM1,THETA1,XM2,THETA2,FN2R,FK2,FNXR,FKX
410 FORMAT(1H F8.1,2F8.3,2(F9.5,F9.3),4F7.4,4F7.2)
      GO TO 450
C   Q NOT 0, COMPUTE P AND A READINGS FOR VALUE OF Q
C   CORRECT Q FOR TILT AND ALINEMENT
420 TQ=TAND(Q+AT+ALQ)
      IF(ABS(DEL).LT.1.0E-6) GO TO 430
      R=(TQ*SIND(DEL-DELC)-SIND(DEL+DELC)/TQ)/2./SIND(DEL)
      TP1=(-R+SQRT(R*R+1))/TC
      TP2=(-R-SQRT(R*R+1))/TC
      P1=ATAND(TP1)+Q-ALP+ALQ
      P2=ATAND(TP2)+Q-ALP+ALQ
      A1=ATAND(REAL(RHO*(TP1*TQ*RHOC-1.))/(TQ+TP1*RHOC))-AT-ALA
      A2=ATAND(REAL(RHO*(TP2*TQ*RHOC-1.))/(TQ+TP2*RHOC))-AT-ALA
      GO TO 440
C   USE LIMITING FORMS OF EQUATIONS FOR DEL NEARLY =0.

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430 P1=Q-ALP+ALQ
    P2=Q-ALP+ALQ-90.
    A1=ATAND(REAL(RHO/TQ))-AT-ALA
    A2=ATAND(REAL(RHO*TQ))-AT-ALA
C   REDUCE ANGLES TO LIE BETWEEN 0 AND 180 DEGREES
440 P1=AMOD(P1+360.,180.)
    A1=AMOD(A1+360.,180.)
    P2=AMOD(P2+360.,180.)
    A2=AMOD(A2+360.,180.)
    WRITE(6,410) D2,DEL,PSI,XM1,THETA1,XM2,THETA2,FN2R,FK2,FXR,
1   FKX,P1,A1,P2,A2
450 D2=D2+DD2
    IF(D2.LT.D2E) GO TO 400
    GO TO 670
C   COMPUTE FILM THICKNESS M=15      CD
C   PICK THICKNESS WITH SMALLEST IMAGINARY PART
455 IF(ABS(AIMAG(T2)).LT.ABS(AIMAG(T1))) GO TO 460
    D2=REAL(T1)
    ERROR=AIMAG(T1)
    K=1
    GO TO 470
460 D2=REAL(T2)
    ERROR=AIMAG(T2)
    K=2
C   COMPUTE DEL AND PSI FOR CALCULATED FILM THICKNESS D2
470 CRP21=RC(RP21,CRP32,FN2*C2*D2/WL)
    CRN21=RC(RN21,CRN32,FN2*C2*D2/WL)
    RHO1=CRP21/CRN21
    PSIX=ATAND(CABS(RHO1))-PSI
    DELX=57.29578*ATAN2(AIMAG(RHO1),REAL(RHO1))-DEL
    DIFN21=REAL(FN2)-FN1
    DIFN32=REAL(FNX(N+1))-REAL(FN2)
C   WEIGHT FRACTION AND WEIGHT OF MATERIAL IN UNIT AREA OF FILM
    FRACTN=DENP/(DENP+(S(REAL(FN2))-S(FNP))*DEN1/(S(FN1)-S(REAL(FN2))))
1 )
    WTM=1.0E-5*D2*FRACTN/(FRACTN/DENP+(1.-FRACTN)/DEN1)
    FN2R=REAL(FN2)
    FXR=REAL(FNX(N+1))
    FK2=-AIMAG(FN2)/REAL(FN2)
    FKX=-AIMAG(FNX(N+1))/REAL(FNX(N+1))
    WRITE(6,480) D2,FN2R,FK2,WTM,DELX,PSIX,ERROR,DIFN21,DIFN32,
1   FRACTN,FXR,FKX,K
480 FORMAT(1H ,F8.1,2F9.5,1PE12.4,0P2F9.3,F12.5,3F10.5,2F9.5,I6)
    GO TO 670
C   CALCULATE SOLUTION FOR N2 FOR FIRST SOLUTION OF QUADRATIC
485 K=1
    GO TO 490
487 K=2
    GO TO 490
489 K=4
C   MX=16 SO THAT SOLN2 WILL PRINT
490 MX=16
    CALL SOLN2
    MX=M
    IF(M.EQ.16 .OR. M.EQ.21 .OR. IS.EQ.1) GO TO (345,347,348,670),K
C   PRINT BLANK SPACE
    WRITE(6,27)
C   CALCULATE ERROR LIMITS FOR N2 AND D2
    DELO=DEL
    PSIO=PSI
    DEL=DELO+1.249*EDEL
    CALL SOLN2

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TN(1)=REAL(FN2)
TD(1)=D2
DEL=DEL0-1.249*EDEL
CALL SOLN2
TN(2)=REAL(FN2)
TD(2)=D2
DEL=DEL0
PSI=PSI0+1.249*EPSI
CALL SOLN2
TN(3)=REAL(FN2)
TD(3)=D2
PSI=PSI0-1.249*EPSI
CALL SOLN2
TN(4)=REAL(FN2)
TD(4)=D2
DEL=DEL0+0.883*EDEL
PSI=PSI0+0.883*EPSI
CALL SOLN2
TN(5)=REAL(FN2)
TD(5)=D2
DEL=DEL0-0.883*EDEL
CALL SOLN2
TN(6)=REAL(FN2)
TD(6)=D2
DEL=DEL0+0.883*EDEL
PSI=PSI0-0.883*EPSI
CALL SOLN2
TN(7)=REAL(FN2)
TD(7)=D2
DEL=DEL0-0.883*EDEL
CALL SOLN2
TN(8)=REAL(FN2)
TD(8)=D2
FN2MIN=AMIN1(TN(1),TN(2),TN(3),TN(4),TN(5),TN(6),TN(7),TN(8))
FN2MAX=AMAX1(TN(1),TN(2),TN(3),TN(4),TN(5),TN(6),TN(7),TN(8))
D2MIN=AMIN1(TD(1),TD(2),TD(3),TD(4),TD(5),TD(6),TD(7),TD(8))
D2MAX=AMAX1(TD(1),TD(2),TD(3),TD(4),TD(5),TD(6),TD(7),TD(8))
WRITE(6,495) D2MIN,D2MAX,FN2MIN,FN2MAX
495 FORMAT(39H0CONFIDENCE LIMITS OF FILM THICKNESS ISF8.1,3H TO F8.1/
1      69H CONFIDENCE LIMITS OF THE REAL PART OF INDEX OF REFRACTI
20N OF FILM ISF12.5,3H TO F12.5)
GO TO (345,347,348,670),K
670 FN2X(1)=FN2X(1)+DFN2(1)
IF(FN2X(1).LT.FN2E(1)) GO TO 343
700 FN2X(2)=FN2X(2)+DFN2(2)
IF(FN2X(2).LT.FN2E(2)) GO TO 342
FNSX(2)=FNSX(2)+DFNS(2)
IF(FNSX(2).LT.FNSE(2)) GO TO 327
FNSX(1)=FNSX(1)+DFNS(1)
IF(FNSX(1).LT.FNSE(1)) GO TO 326
WL=WL+DWL
IF(WL.LT.WLE) GO TO 320
705 AI=AI+DAI
IF(AI.LT.AIE) GO TO 312
FN1=FN1+DFN1
IF(FN1.LT.FN1E) GO TO 311
GO TO 20
C      CALCULATE REFRACTIVE INDEX OF SUBSTRATE CNS
710 FNS=FN1*S1/C1*CSQRT(1.-4.*RHO*S1**2/(RHO+1.))**2)
FNSI(1)=REAL(FNS)
FNSI(2)=-AIMAG(FNS)/FNSI(1)
FNSE(1)=0.

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      FNSE(2)=0.
      WRITE(6,720) FNSI,DEL,PSI
720  FORMAT(20H0INDEX OF SUBSTRATE=F9.4,F9.4,2H ,2X,4HDEL=,
      1 F9.3,2X,4HPSI=F9.3)
      IF(FNSI(2).LT.0.) GO TO 725
      GO TO 705
725  WRITE(6,727)
727  FORMAT(62H0KAPPA IS SET EQUAL TO 0,SINCE A NEGATIVE VALUE WAS CALC
      1ULATED)
      FNSI(2)=0.
      GO TO 705
C     COMPUTE CONSTANTS OF WAVE PLATE           CWP
C     ASSUMES ANGLE OF TILT AT IS ZERO
730  Z1=Z1+ALP
      Z2=Z2+ALA
      Z3=Z3+ALP
      Z4=Z4+ALA
      Z5=Z5+ALQ
      WRITE(6,27) L,Z1,Z2,Z3,Z4,Z5
      IF(ABS(Z3-Z5).LT.0.1 .OR. ABS(Z1-Z5).LT.0.1) GO TO 745
735  B=(TAND(Z2)*(TAND(Z3-Z5)*TAND(Z5)-TAND(Z1-Z5)/TAND(Z5))-TAND(Z4)*
      1 (TAND(Z1-Z5)*TAND(Z5)-TAND(Z3-Z5)/TAND(Z5)))/2./
      2 (TAND(Z2)-TAND(Z4))
      DELC= ATAN2(SQRT(-B*B-TAND(Z1-Z5)*TAND(Z3-Z5)),B)*57.29578
      TC=1./SQRT(-TAND(Z1-Z5)*TAND(Z3-Z5))
      RHOC=TC*CEXP((0.,-1.)*DELC/57.29578)
      RHO =TAND(Z2)*(TAND(Z5)+TAND(Z1-Z5)*RHOC)/(TAND(Z1-Z5)*TAND(Z5)*
      1 RHOC-1.)
      DEL=57.29578*ATAN2(AIMAG(RHO),REAL(RHO))
      PSI=ATAND(CABS(RHO))
      WRITE(6,740) TC,DELC,DEL,PSI
740  FORMAT(4H TC=,F10.5,9H DELTA C=,F10.5,7H DELTA=,F15.5,5H PSI=,
      1 F15.5)
      GO TO 20
745  WRITE (6,747)
747  FORMAT( 73H0CONSTANTS OF WAVE PLATE CAN NOT BE ACCURATELY CALCULAT
      1ED FROM ABOVE DATA)
      GO TO 20
C     CALCULATE ANGLE OF TILT OF STAGE ON ELLIPSOMETER CAT IS COMP
C     ANGLE WITH REAL PART ANGLE AND IMAGINARY PART ERROR
750  Z1=Z1+ALP
      Z2=Z2+ALA
      Z3=Z3+ALP
      Z4=Z4+ALA
      Z5=Z5+ALQ
      WRITE(6,27 ) L,Z1,Z2,Z3,Z4,Z5
      TP1=TAND(Z1-Z5)
      TA1=TAND(Z2)
      TP2=TAND(Z3-Z5)
      TA2=TAND(Z4)
      TQ =TAND(Z5)
      ALP1=TA1*(TQ+TP1*RHOC)
      ALP2=TA2*(TQ+TP2*RHOC)
      GAM1=TP1*TQ*RHOC-1.
      GAM2=TP2*TQ*RHOC-1.
      BET1=ALP1/SIND(Z2)/COSD(Z2)+(TA1-ALP1*TP1*RHOC/GAM1)/COSD(Z5)**2
      BET2=ALP2/SIND(Z4)/COSD(Z4)+(TA2-ALP2*TP2*RHOC/GAM2)/COSD(Z5)**2
      CAT=(ALP2*GAM1-ALP1*GAM2)/(BET1*GAM2-BET2*GAM1)*57.29578
      ATX=REAL(CAT)
      Z1=Z1+ATX
      Z2=Z2+ATX
      Z3=Z3+ATX

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      Z4=Z4+ATX
      Z5=Z5+ATX
C      COMPUTE RHO,DEL,PSI
      GO TO 174
755 PRINT 760,CAT,DEL,PSI
760 FORMAT(15H ANGLE OF TILT=,F13.5,15H DEGREES,ERROR=,F13.5,
1       7H DELTA=,F15.5,5H PSI=,F15.5)
      IF(M.EQ.26) ATX=(ATX+AT)/2.
      AT=ATX
      GO TO 20
810 STOP
C INSTRUCTION CNK M=31 COMPUTES N AND KAPPA OF FILM
850 D2=D2I
852 PRINT 855,D2
855 FORMAT(1H0,90X,F15.1)
860 CALL MIN2V(FN2I(1),DFN2(1),FN2E(1),FN2I(2),DFN2(2),FN2E(2))
      D2=D2+DD2
      IF(D2.LT.D2E) GO TO 852
      GO TO 20
      END

SUBROUTINE SOLN2
C      SOLVES FOR REAL PART OF REFRACTIVE INDEX AND THICKNESS OF
C      A FILM FOR MEASUREMENTS OF DELTA AND PSI
C      ER2 IS ERROR OF SOLUTION,THICK IS FILM THICKNESS,INDEX IN FN2
C      IF K=1 OR 3, FIRST(POSITIVE SIGN) SOLUTION IS USED
C      IF K=2 OR 4, SECOND(NEGATIVE SIGN) SOLUTION IS USED
      COMMON FN1,S1,C1,N,FNX(900),D(900),FN2,CRP,CRN,CRP32,CRN32,WL,
1 RP21,RN21,DEL,PSI,C2,C3,FN2I(2),DFN2(2),FN2E(2),FN2X(2),T1,T2,T3,
2 T4,D2,DELX,PSIX,ELDEL,ELPSI,DENP,FNP,DEN1,M,K,IS
      COMPLEX FNX,FN2,CRP,CRN,CRP32,CRN32,RP21,RN21,C2,C3,T1,T2,T3,T4,
1 T5,T6,RHO,RC
C      S IS USED FOR CALCULATING SPECIFIC REFRACTION
      S(XN)=(XN*XN-1.)/(XN*XN+2.)
      ATAND(X)=ATAN(X)*57.29578
      X1=FN2X(1)
      X3=FN2X(1)+DFN2(1)
      GO TO (10,20,10,20),K
10 ER1=AIMAG(T1)
   ER3=AIMAG(T3)
   GO TO 30
20 ER1=AIMAG(T2)
   ER3=AIMAG(T4)
30 DO 80 I=1,20
      X2=(X1+X3)/2.
      FN2=CMPLX(X2,-FN2X(2)*X2)
      CALL CRC
      CALL CALDX(T5,T6)
      GO TO (40,50,40,50),K
40 D2=REAL(T5)
   ER2=AIMAG(T5)
   GO TO 60
50 D2=REAL(T6)
   ER2=AIMAG(T6)
C      COMPUTE DEL AND PSI FOR FILM THICKNESS D2
60 RHO=RC(RP21,CRP32,FN2*C2*D2/WL)/RC(RN21,CRN32,FN2*C2*D2/WL)
   DELX =ATAN2(AIMAG(RHO),REAL(RHO))*57.29578-DEL
   PSIX=ATAND(CABS(RHO))-PSI
   IF(ABS(DELX).LT.ELDEL.AND.ABS(PSIX).LT.ELPSI) GO TO 100
C      HAS NOT CONVERGED TO ELDEL AND ELPSI. CHANGE LIMITS X1,X3
C      IF ER1 AND ER2 HAVE SAME SIGN,X1=X2 AND ER1=ER2,OTHERWISE
C      ER2 AND ER3 HAVE SAME SIGN,X3=X2 AND ER3=ER2

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      IF((ER1.GT.0.0 .AND. ER2.GT.0.0).OR.(ER1.LT.0.0 .AND.
1  ER2.LT.0.0)) GO TO 70
      X3=X2
      ER3=ER2
      GO TO 80
70  X1=X2
      ER1=ER2
80  CONTINUE
90  D2=1.0E30
      FN2=1.0E30
      RETURN
C  IF FILM THICKNESS D2 IS NEGATIVE,TREAT AS NO SOLUTION
100 IF(D2.LT.0.) GO TO 90
C  PRINT SOLUTION AND ERROR LIMITS
      IF(M.EQ.17 .OR. M.EQ.22) GO TO 120
      DIFN21=X2-FN1
      DIFN32=REAL(FNX(N+1))-X2
      FRACTN=DENP/(DENP+(S(X2)-S(FNP))*DEN1/(S(FN1)-S(X2)))
      WTMT=1.0E-5*D2*FRACTN/(FRACTN/DENP+(1.-FRACTN)/DEN1)
      FN2R=REAL(FN2)
      FNXR=REAL(FNX(N+1))
      FK2=-AIMAG(FN2)/REAL(FN2)
      FKX=-AIMAG(FNX(N+1))/REAL(FNX(N+1))
      PRINT 110,D2,FN2R,FK2,WTMT,DELX,PSIX,ER2,DIFN21,DIFN32,
1  FRACTN,FNXR,FKX,K
110 FORMAT(1H ,F8.1,2F9.5,1PE12.4,0P2F9.3,F12.5,3F10.5,2F9.5,I6)
      IS=2
120 RETURN
      END

      SUBROUTINE CRC
C  CALCULATES CRP32 AND CRN32 REFLECTION COEF OF MEDIUM 2 AND 3
      COMMON FN1,S1,C1,N,FNX(900),D(900),FN2,CRP,CRN,CRP32,CRN32,WL,
1  RP21,RN21,DEL,PSI,C2,C3,FN2I(2),DFN2(2),FN2E(2),FN2X(2),T1,T2,T3,
2  T4,D2,DELDX,PSIDX, ERDEL,ERPSI,DENP,FNP,DEN1
      COMPLEX FNX,FN2,CRP,CRN,CRP32,CRN32,RP21,RN21,C2,C3,T1,T2,T3,T4
      COMPLEX RC,RP32,RN32
      SRC(A,B)=(A-B)/(A+B)
      X=FN1*S1
      C2=CSQRT(1.-(X/FN2)**2)
      C3=CSQRT(1.-(X/FNX(3))**2)
      RP21=SRC(FN2*C1,FN1*C2)
      RN21=SRC(FN1*C1,FN2*C2)
      IF(N.EQ.2) GO TO 10
      RP32=SRC(FNX(3)*C2,FN2*C3)
      RN32=SRC(FN2*C2,FNX(3)*C3)
      CRP32=RC(RP32,CRP,FNX(3)*C3*D(3)/WL)
      CRN32=RC(RN32,CRN,FNX(3)*C3*D(3)/WL)
      RETURN
10  CRP32=SRC(FNX(3)*C2,FN2*C3)
      CRN32=SRC(FN2*C2,FNX(3)*C3)
      RETURN
      END

      COMPLEX FUNCTION RC(R21,CR32,Q )
C  RC=REFLECTION COEFFICIENT INCLUDING EFFECT OF UNDERLYING LAYERS
C  FOLLOWING CARD IS REQUIRED FOR FORTRAN V ONLY
      COMPLEX CEXP,CLOG,CSQRT
      COMPLEX R21,CR32,Q ,T
      T=CEXP((0.,-12.56637)*Q)
C  Q=N2*COS(PHI2)*D/WL (0.,-12.56637)=-4*PI*J
      RC=(R21+CR32*T)/(1.+R21*CR32*T)

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RETURN  
END

SUBROUTINE CALDX(D2C1,D2C2)

C FOLLOWING CARD IS REQUIRED FOR FORTRAN V ONLY  
COMPLEX CEXP,CLOG,CSQRT  
C CALCULATES FILM THICKNESS AND ERROR TERMS  
COMMON FN1,S1,C1,N,FNX(900),D(900),FN2,CRP,CRN,CRP32,CRN32,WL,  
1 RP21,RN21,DEL,PSI,C2,C3,FN2I(2),DFN2(2),FN2E(2),FN2X(2),T1,T2,T3,  
2 T4,D2,DELDX,PSIDX, ERDEL,ERPSI,DENP,FNP,DEN1,M,K  
COMPLEX FNX,FN2,CRP,CRN,CRP32,CRN32,RP21,RN21,C2,C3,T1,T2,T3,T4  
COMPLEX E,B,C,Y1,Y2,D2C1,D2C2,RHO,T5,T6  
RHO=SIN(PSI/57.29578)/COS(PSI/57.29578)\*CEXP((0.,1.)\*DEL/57.29578)  
C Y=EXP(-2 J DEL2) LET E\*Y\*\*2+BY+C=0 Y1,Y2 ARE TWO SOLUTIONS  
E=RHO\*RP21\*CRP32\*CRN32-RN21\*CRP32\*CRN32  
B=RHO\*(CRN32+RP21\*RN21\*CRP32)-CRP32-RP21\*RN21\*CRN32  
C=RHO\*RN21-RP21  
T5=CSQRT(B\*\*2-4.\*E\*C)  
GO TO (20,20,10,10),K  
C MAKE IMAGINARY PART OF SQUARE ROOT POSITIVE  
10 IF(AIMAG(T5).LT.0.) T5=-T5  
20 Y1=(-B+T5)/2./E  
Y2=(-B-T5)/2./E  
T5=CLOG(Y1)  
T6=CLOG(Y2)  
D2C1=WL\*T5/(0.,-12.56637)/FN2/C2  
D2C2=WL\*T6/(0.,-12.56637)/FN2/C2  
RETURN  
END

SUBROUTINE MIN2V(XI,DX,XF,YI,DY,YF)

C USES FUNCTION FUNC(X,Y) WHICH MUST BE INCLUDED. DETERMINES AND PRINTS  
C VALUES OF X BETWEEN XI AND XF AND VALUES OF Y BETWEEN YI AND YF THAT  
C MINIMIZE FUNC. WILL FIND MULTIPLE MINIMUMS IF THEY ARE SEPARATED  
C BY MORE THAN DX AND DY  
DIMENSION F(50,50)  
COMMON FN1,S1,C1,N,FNX(900),D(900),FN2,CRP,CRN,CRP32,CRN32,WL,  
1 RP21,RN21,DEL,PSI,C2,C3,FN2I(2),DFN2(2),FN2E(2),FN2X(2),T1,T2,T3,  
2 T4,D2,DELDX,PSIDX, ERDEL,ERPSI,DENP,FNP,DEN1,MX,K,IS,RHO  
COMPLEX FNX,FN2,CRP,CRN,CRP32,CRN32,RP21,RN21,C2,C3,T1,T2,T3,T4  
COMPLEX RC,RHO  
C COMPUTE NUMBER OF VALUES OF X AND Y FOR RANGES XI-DX TO XF+DX  
C AND YI-DY TO YF+DY.  
NX=(1.000001\*XF-XI)/DX+3  
NY=(1.000001\*YF-YI)/DY+3  
IF(NX.GT.50) PRINT 10,DX  
10 FORMAT('0 INCREMENT OF X,'E12.5,' IS TOO SMALL')  
IF(NY.GT.50) PRINT 20,DY  
20 FORMAT('0 INCREMENT OF Y,'E12.5,' IS TOO SMALL')  
C COMPUTE INITIAL VALUE OF X  
X=XI-DX  
C COMPUTE TABLE F OF FUNCTION FUNC  
DO 40 I=1,NX  
Y=YI-DY  
DO 30 J=1,NY  
F(I,J)=FUNC(X,Y)  
C\*\*\*\*\*DIAGNOSTIC PRINTING\*\*\*\*\*  
C PRINT 35,I,J,F(I,J)  
30 Y=Y+DY  
35 FORMAT(2I5,E20.7)  
40 X=X+DX  
NX1=NX-1

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NY1=NY-1
DO 910 I=2,NX1
DO 900 J=2,NY1
C SEARCH FOR MINIMUMS OF F (VALUES LESS THAN ALL 8 SURROUNDING VALUES)
  IF(F(I,J).LT.F(I-1,J-1).AND. F(I,J).LT.F(I-1,J) .AND.
1  F(I,J).LT.F(I-1,J+1) .AND. F(I,J).LT.F(I,J-1) .AND.
2  F(I,J).LT.F(I,J+1) .AND. F(I,J).LT.F(I+1,J-1)
3  .AND. F(I,J).LT.F(I+1,J) .AND.
4  F(I,J).LT.F(I+1,J+1))GO TO 50
  GO TO 900
50  XMIN=XI+(I-2)*DX
    YMIN=YI+(J-2)*DY
    FMIN=F(I,J)
C A MINIMUM FMIN OCCURS NEAR POINT I,J AT XMIN-DX TO XMIN+DX AND
C YMIN-DY TO YMIN+DY,
C SUBDIVIDE RANGE TO LOCATE MINIMUM.
  XD=DX/2
  YD=DY/2
C SUBDIVIDE RANGE 10 TIMES
  DO 550 K=1,10
    F13=FUNC(XMIN-XD,YMIN-YD)
    F14=FUNC(XMIN,YMIN-YD)
    IF(F13.LT.FMIN) GO TO 110
    IF(F14.LT.FMIN) GO TO 120
C F14 GT FMIN
105 F15=FUNC(XMIN+XD,YMIN-YD)
    IF(F15.LT.FMIN) GO TO 130
C F15 GT FMIN
107 F18=FUNC(XMIN+XD,YMIN)
    IF(F18.LT.FMIN) GO TO 140
    F22=FUNC(XMIN+XD,YMIN+YD)
    IF(F22.LT.FMIN) GO TO 150
C F22 GT FMIN
    F21=FUNC(XMIN,YMIN+YD)
    IF(F21.LT.FMIN) GO TO 160
C F21 GT FMIN
    F20=FUNC(XMIN-XD,YMIN+YD)
    IF(F20.LT.FMIN) GO TO 170
    F17=FUNC(XMIN-XD,YMIN)
    IF(F17.LT.FMIN) GO TO 180
C FMIN LT SURROUNDINGS
    GO TO 500
110 IF(F14.LT.F13) GO TO 120
C F13 LT F14 AND FMIN
    F17=FUNC(XMIN-XD,YMIN)
C IF F17 LT F13, CONTINUE SCAN WITH F15
    IF(F17.LT.F13) GO TO 105
C F13 LT F14,FMIN,F17
    F12=FUNC(XMIN-2*XD,YMIN-YD)
    IF(F12.LT.F13) GO TO 190
    F10=FUNC(XMIN-XD,YMIN-2*YD)
    IF(F10.LT.F13) GO TO 200
C F13 IS NEW MINIMUM
    FMIN=F13
    XMIN=XMIN-XD
    YMIN=YMIN-YD
    GO TO 500
C F14 LT FMIN,F13
120 F15=FUNC(XMIN+XD,YMIN-YD)
    IF(F15.LT.F14) GO TO 130
    F11=FUNC(XMIN+XD,YMIN-2*YD)
    IF(F11.LT.F14) GO TO 210

```



```

        F10=FUNC(XMIN-XD,YMIN-2*YD)
        IF(F10.LT.F14) GO TO 200
        F17=FUNC(XMIN-XD,YMIN)
        IF(F17.LT.F14) GO TO 107
        F18=FUNC(XMIN+XD,YMIN)
        IF(F18.LT.F14) GO TO 140
C      F14 IS NEW MINIMUM
        FMIN=F14
        YMIN=YMIN-YD
        GO TO 500
C      F15 LT FMIN ,F14
130    F11=FUNC(XMIN+XD,YMIN-2*YD)
        IF(F11.LT.F15) GO TO 210
        F18=FUNC(XMIN+XD,YMIN)
        IF(F18.LT.F15) GO TO 140
        F16=FUNC(XMIN+2*XD,YMIN-YD)
        IF(F16.LT.F15) GO TO 220
C      F15 IS NEW MINIMUM
        FMIN=F15
        XMIN=XMIN+XD
        YMIN=YMIN-YD
        GO TO 500
C      F18 LT FMIN,F15,F14
140    F16=FUNC(XMIN+2*XD,YMIN-YD)
        IF(F16.LT.F18) GO TO 220
        F22=FUNC(XMIN+XD,YMIN+YD)
        IF(F22.LT.F18) GO TO 150
        F21=FUNC(XMIN,YMIN+YD)
        IF(F21.LT.F18) GO TO 160
        F23=FUNC(XMIN+2*XD,YMIN+YD)
        IF(F23.LT.F18) GO TO 230
C      F18 IS NEW MINIMUM
        FMIN=F18
        XMIN=XMIN+XD
        GO TO 500
C      F22 LT FMIN,F18
150    F21=FUNC(XMIN,YMIN+YD)
        IF(F21.LT.F22) GO TO 160
        F23=FUNC(XMIN+2*XD,YMIN+YD)
        IF(F23.LT.F22) GO TO 230
        F25=FUNC(XMIN+XD,YMIN+2*XD)
        IF(F25.LT.F22) GO TO 240
C      F22 IS NEW MINIMUM
        FMIN=F22
        XMIN=XMIN+XD
        YMIN=YMIN+YD
        GO TO 500
C      F21 LT FMIN,F22,F18
160    F25=FUNC(XMIN+XD,YMIN+2*XD)
        IF(F25.LT.F21) GO TO 240
        F20=FUNC(XMIN-XD,YMIN+YD)
        IF(F20.LT.F21) GO TO 170
        F17=FUNC(XMIN-XD,YMIN)
        IF(F17.LT.F21) GO TO 180
        F24=FUNC(XMIN-XD,YMIN+2*YD)
        IF(F24.LT.F21) GO TO 250
C      F21 IS NEW MINIMUM
        FMIN=F21
        YMIN=YMIN+YD
        GO TO 500
C      F20 LT FMIN,F21
170    F17=FUNC(XMIN-XD,YMIN)

```

```

IF(F17.LT.F20) GO TO 180
F24=FUNC(XMIN-XD,YMIN+2*YD)
IF(F24.LT.F20) GO TO 250
F19=FUNC(XMIN-2*XD,YMIN+YD)
IF(F19.LT.F20) GO TO 260
C   F20 IS NEW MINIMUM
      FMIN=F20
      XMIN=XMIN-XD
      YMIN=YMIN+YD
      GO TO 500
C   F17 LT FMIN F20,F21,F13,F14
180  F12=FUNC(XMIN-2*XD,YMIN-YD)
      IF(F12.LT.F17) GO TO 190
      F19=FUNC(XMIN-2*XD,YMIN+YD)
      IF(F19.LT.F17) GO TO 260
C   F17 IS NEW MINIMUM
      FMIN=F17
      XMIN=XMIN-XD
      GO TO 500
C   F12 LT F13,FMIN,F17
190  F10=FUNC(XMIN-XD,YMIN-2*YD)
      IF(F10.LT.F12) GO TO 200
      FMIN=F12
      XMIN=XMIN-2*XD
      YMIN=YMIN-YD
192  FX=FUNC(XMIN-XD,YMIN-YD)
      IF(FMIN.GT.FX) GO TO 194
      FX=FUNC(XMIN-XD,YMIN)
      IF(FMIN.GT.FX) GO TO 196
      FX=FUNC(XMIN-XD,YMIN+YD)
      IF(FMIN.GT.FX) GO TO 198
      GO TO 500
194  YMIN=YMIN-YD
196  XMIN=XMIN-XD
      FMIN=FX
      GO TO 300
198  YMIN=YMIN+YD
      GO TO 196
C   F10 LT F13,F14,F12,FMIN
200  FMIN=F10
C   CHECK TO SEE THAT F10 IS NEW MINIMUM
      XMIN=XMIN-XD
      YMIN=YMIN-2*YD
202  FX=FUNC(XMIN-XD,YMIN-YD)
      IF(FMIN.GT.FX) GO TO 204
      FX=FUNC(XMIN,YMIN-YD)
      IF(FMIN.GT.FX) GO TO 206
      FX=FUNC(XMIN+XD,YMIN-YD)
      IF(FMIN.GT.FX) GO TO 208
      GO TO 500
204  XMIN=XMIN-XD
206  YMIN=YMIN-YD
      FMIN=FX
      GO TO 300
208  XMIN=XMIN+XD
      GO TO 206
C   F11 LT F14,F15
210  F18=FUNC(XMIN+XD,YMIN)
      IF(F18.LT.F11) GO TO 140
      F16=FUNC(XMIN+2*XD,YMIN-YD)
      IF(F16.LT.F11) GO TO 220
      FMIN=F11

```

```

XMIN=XMIN+XD
YMIN=YMIN-2*YD
GO TO 202
C   F16 LT F15,F11,F18
220   FMIN=F16
      XMIN=XMIN+2*XD
      YMIN=YMIN-YD
222   FX=FUNC(XMIN+XD,YMIN-YD)
      IF(FMIN.GT.FX) GO TO 224
      FX=FUNC(XMIN+XD,YMIN)
      IF(FMIN.GT.FX) GO TO 226
      FX=FUNC(XMIN+XD,YMIN+YD)
      IF(FMIN.GT.FX) GO TO 228
      GO TO 500
224   YMIN=YMIN-YD
226   XMIN=XMIN+XD
      FMIN=FX
      GO TO 300
228   YMIN=YMIN+YD
      GO TO 226
C   F23 LT F18,F22,FMIN
230   F25=FUNC(XMIN+XD,YMIN+2*XD)
      IF(F25.LT.F23) GO TO 240
      FMIN=F23
      XMIN=XMIN+2*XD
      YMIN=YMIN+YD
      GO TO 222
C   F25 LT F21,F22,F23,FMIN
240   FMIN=F25
      XMIN=XMIN+XD
      YMIN=YMIN+2*YD
242   FX=FUNC(XMIN-XD,YMIN+YD)
      IF(FMIN.GT.FX) GO TO 244
      FX=FUNC(XMIN,YMIN+YD)
      IF(FMIN.GT.FX) GO TO 226
      FX=FUNC(XMIN+XD,YMIN+YD)
      IF(FMIN.GT.FX) GO TO 248
      GO TO 500
244   XMIN=XMIN-XD
246   YMIN=YMIN+YD
      FMIN=FX
      GO TO 300
248   XMIN=XMIN+XD
      GO TO 246
C   F24 LT F21,F20,F17,FMIN
250   F19=FUNC(XMIN-2*XD,YMIN+YD)
      IF(F19.LT.F24) GO TO 260
      FMIN=F24
      XMIN=XMIN-XD
      YMIN=YMIN+2*YD
      GO TO 242
C   F19 LT F20,F17,FMIN
260   F17=FUNC(XMIN-XD,YMIN)
      IF(F17.LT.F19) GO TO 180
      FMIN=F19
      XMIN=XMIN-2*XD
      YMIN=YMIN+YD
      GO TO 192
C   FOLLOW MINIMUM FOR 5 STEPS
300   DO 400 KK=1,5
      FX=FUNC(XMIN-XD,YMIN-YD)
      IF(FX.LT.FMIN) GO TO 310

```

```

        FX=FUNC(XMIN-XD,YMIN)
        IF(FX.LT.FMIN) GO TO 320
        FX=FUNC(XMIN-XD,YMIN+YD)
        IF(FX.LT.FMIN) GO TO 330
        FX=FUNC(XMIN,YMIN-YD)
        IF(FX.LT.FMIN) GO TO 340
        FX=FUNC(XMIN,YMIN+YD)
        IF(FX.LT.FMIN) GO TO 350
        FX=FUNC(XMIN+XD,YMIN-YD)
        IF(FX.LT.FMIN) GO TO 360
        FX=FUNC(XMIN+XD,YMIN)
        IF(FX.LT.FMIN) GO TO 370
        FX=FUNC(XMIN+XD,YMIN+XD)
        IF(FX.LT.FMIN) GO TO 380
        GO TO 500
310     YMIN=YMIN-YD
320     XMIN=XMIN-XD
        GO TO 400
330     YMIN=YMIN+YD
        GO TO 320
340     YMIN=YMIN-YD
        GO TO 400
350     YMIN=YMIN+YD
        GO TO 400
360     YMIN=YMIN-YD
370     XMIN=XMIN+XD
        GO TO 400
380     YMIN=YMIN+YD
        GO TO 370
400     FMIN=FX
C       A MINIMUM IS NOT FOUND IN 5 STEPS
        GO TO 600
500     XD=XD/2
        YD=YD/2
550     CONTINUE
C       NEW MINIMUM IS FOUND
        GO TO 700
560     FORMAT(5E15.6,3I5/(7F15.6))
600     PRINT 610,K,FMIN,XMIN,YMIN,XD,YD
610     FORMAT('0 ITERATION NUMBER' I3,' FAILED FOR MINIMUM'E12.5,' AT X
1='E12.5,' Y='E12.5,' RANGES =' 2E12.5)
C*****PRINT VALUES AT MINIMUM
700     FN2=CMPLX(XMIN,-XMIN*YMIN)
        T1=RC(RP21,CRP32, FN2*C2*D2/WL)/RC(RN21,CRN32, FN2*C2*D2/WL)
        DDEL=ATAN2(AIMAG(T1),REAL(T1))*57.29578-DEL
        DPSI=ATAN(ABS(T1))*57.29578-PSI
        XD=2*XD
        YD=2*YD
        PRINT 800, XMIN,YMIN,XD,YD,FMIN,DDEL,DPSI
800     FORMAT(' 5F15.5,2F10.3)
900     CONTINUE
910     CONTINUE
        RETURN
        END

FUNCTION FUNC(FRN,FK)
C     COMPUTES VALUES OF DELTA AND PSI, DELC AND PSIC, FOR A FILM
C     OF N=FRN,KAPPA=FK, AND THICKNESS=D2 AND ERROR TERM, FUNC
COMMON FN1,S1,C1,N, FN1(900), D(900), FN2,CRP,CRN,CRP32,CRN32,WL,
1 RP21,RN21,DEL,PSI,C2,C3, FN2I(2),DFN2(2),FN2E(2),FN2X(2),T1,T2,T3,
2 T4,O2,DELDX,PSIDX, ERDEL,ERPSI,DENP,FNP,DEN1,MX,K,IS,RHO
COMPLEX FN1, FN2,CRP,CRN,CRP32,CRN32,RP21,RN21,C2,C3,T1,T2,T3,T4

```



```
COMPLEX RC,RHO
  FN2=CMPLX(FRN,-FRN*FK)
  CALL CRC
  FUNC=ABS(RC(RP21,CRP32, FN2*C2*D2/WL)/RC(RN21,CRN32, FN2*C2*D2/WL)
1  -RHO)
  RETURN
  END
```

## 4.2. Subprograms

<u>Subprogram</u>	<u>Type</u>	
ABS	Real	Absolute value
AIMAG	Real	Imaginary part of complex argument
AMAX1	Real	Maximum of real arguments
AMIN1	Real	Minimum of real arguments
AMØD	Real	Remainder obtained by dividing first by second argument.
ATAN	Real	Arctangent
ATAN2	Real	Divides first by second argument and calculates arctangent of quotient in proper quadrant.
ATAND	Real	Arctangent given in degrees, statement function
CALDX		Subroutine furnished with program. Calculates two complex values (D2C1 and D2C2) for the thickness of the top film for DEL and PSI given in common. Requires CRN, CRP, CRN32, CRP32, RN21, and RP21, to have been previously calculated. The value of K determines which solution corresponds to D2C1 and D2C2.
CABS	Real	Absolute value of complex argument
CEXP	Complex	Complex exponential
CLØG	Complex	Complex natural logarithm
CMPLX	Complex	Calculates a complex number. The real part of the complex number is the first argument and imaginary part is the second argument.
CØS	Real	Cosine
CØSD	Real	Cosine of angle in degrees, statement function.
CRC		Subroutine furnished with program. Computes C2, C3, RP21, RN21, CRN32, and CRP32.
CSQRT	Complex	Complex square root

MAXO	Integer	Result is the maximum of the integer arguments.
RC	Complex	Complex function furnished with program. Computes the reflection coefficient from a surface covered by one or many films. Requires the Fresnel reflection coefficient (R21) from the top film, the reflection coefficient (CR32) from the medium under the top film, i.e., either the Fresnel reflection coefficient of the substrate or the reflection coefficient from the second film considering underlying films, and $Q = n_f \cos \varphi_f d_f / \lambda$ where $n_f$ , $\varphi_f$ , and $d_f$ are the refractive index, angle of reflection, and thickness of film.
REAL	Real	The real part of a complex number.
S	Real	Statement function
SIN	Real	Sine
SIND	Real	Statement function. The sine of an angle given in degrees.
SOLN2		Subroutine furnished by program. Solves by a search procedure for both the real part of the refractive index and thickness of the top film on a surface that will give values of DELX and PSIX ( $\Delta$ and $\psi$ ) that will agree with given values DEL and PSI within tolerance ELDEL and ELPSI. The solution will be printed unless MX=17 or 22. The real part of the refractive index of the film is assumed to lie between FN2X(1) and FN2X(1)+DFN2(1) and the value of kappa of the film is FN2X(2). The solution to be used for the thickness of the film is determined by the value of $\kappa$ . The complex thicknesses of the film and the limits of the range of refractive index to be searched, i.e., at FN2X(1) and FN2X(1)+DFN2(1) must have been calculated and stored in T1, T2, T3, and T4.
SQRT	Real	If a solution is printed, IS is made equal to 2. The search procedure is described in Section 3.5.
SRC	Complex	Square root
TAND	Real	Statement function used in computing Fresnel reflection coefficients. Statement function. The tangent of an angle given in degrees.

#### 4.3. Variables Used in Program

##### a. Variables in Common

<u>Fortran</u>	<u>Type</u>	
C1	Real	$\cos\phi_1$ Cosine of angle of incidence
C2	Complex	$\cos\phi_2$ Cosine of angle of refraction in top film
C3	Complex	$\cos\phi_3$ Cosine of angle of refraction in 2nd medium
CRN	Complex	$R^n$ Total reflection coefficient for light polarized normal to the plane of incidence.
CRP	Complex	$R^p$ Total reflection coefficient for light polarized parallel to the plane of incidence.
CRN32	Complex	$R_{32}^n$ Total reflection coefficient between mediums 2 and 3.
CRP32	Complex	$R_{32}^p$ Total reflection coefficient between mediums 2 and 3.
D(900)	Real	$d_1$ Thicknesses of films
D2	Real	$d_2$ Thickness of top film
DEL	Real	$\Delta$ Relative phase retardation
DENI	Real	$\rho_1$ Density of medium 1
DENP	Real	$\rho_p$ Density of medium p
DFN2(2)	Real	$\delta n_2$ Increments for film refractive index
ELDEL	Real	Error limits for $\Delta$
ELPSI	Real	Error limits for $\psi$
FN1	Real	$n_1$ Refractive index of medium
FN2	Complex	$\hat{n}_f$ or $\hat{n}_2$ Refractive index of top film
FN2E(2)	Real	Final values to be used for refractive index of top film.
FN2I(2)	Real	Initial values to be used for refractive index of top film.



FNZX(2)	Real		Refractive index of top film. The complex refractive index (FN2) is computed from FN2X.
FNX(900)	Complex	$n_1$	Refractive index of films other than top film and of the substrate.
FNP	Real	$n_p$	Refractive index of material in film.
IS	Integer		IS determines if a solution for refractive index of the film has been found by SØLN2. It is originally equal to 1, and is changed to 2 when a solution is found.
K	Integer		In calculating the thickness of a film, two solutions are obtained (see Section 3.4). K identifies the solution used, being 1 for the positive solution given by eq. 22 and 2 for the negative solution given by eq. 23. The square root of ( $B^2-4EC$ ) is taken so that the real part of the square root is positive. In searching for the refractive index of the film in subroutine SØLN2, if no solution is found for either K=1 or 2 (using either eq. 22 or 23), the square root of ( $B^2-4EC$ ) is taken so the imaginary part is positive. In some cases, a solution will then be found for the refractive index of the film which is labeled K=3 or 4 corresponding to eq. 22 or 23, respectively.
MX	Integer		Used in SØLN2 to control printing. The solution is printed unless MX=17 or 22. Generally, MX is equal to M.
N	Integer		The number of films on the surface plus 1. Initially, N=2 corresponding to one film.
PSI	Real	$\psi$	$\tan \psi$ is relative reflection coefficient.
PSIX	Complex	$\delta\psi$	Error in $\psi$
RP21	Complex	$r_{21}^p$	Fresnel reflection coefficient between medium and film next to medium for light polarized parallel to the plane of incidence.

<u>Fortran</u>	<u>Type</u>	
RN21	Real	$r_{21}^n$ Fresnel reflection coefficient between medium and film next to medium for light polarized normal to the plane of incidence.
S1	Real	$\sin\phi_1$ Sine of angle of incidence
T1, T2, T3, T4	Complex	Temporary storage
WL	Real	$\lambda$ Vacuum wavelength of light
b. Complex Variables Not in Common		
ALP1		$\alpha_1$ See Section 3.3
ALP2		$\alpha_2$ See Section 3.3
BET1		$\beta_1$ See Section 3.3
BET2		$\beta_2$ See Section 3.3
C2		$\cos\phi_2$ Cosine of angle of refraction in top film
C3		$\cos\phi_3$ Cosine of angle of refraction in film or substrate adjacent to top film.
CAT		Complex angle of tilt. See Section 3.3.
CI		$\cos\phi_1$ Cosine of angle of refraction in medium i.
CIP1		$\cos\phi_{i+1}$ Cosine of angle of refraction in medium i+1.
CN		$\cos\phi_n$ Cosine of angle of refraction in the substrate.
CNM1		$\cos\phi_{n-1}$ Cosine of angle of refraction in the film adjacent to the substrate.
CRN		$R^n$ Reflection coefficient for normal polarization considering underlying films.

CRN21	$R_{21}^n$	Reflection coefficient from top film for normal polarization considering underlying films.
CRN32	$R_{32}^n$	Reflection coefficient from second film or substrate for normal polarization considering underlying layers.
CRP	$R^p$	Reflection coefficient for parallel polarization considering underlying films.
CRP21	$R_{21}^p$	Reflection coefficient from top film for parallel polarization considering underlying layers.
CRP32	$R_{32}^p$	Reflection coefficient from second film or substrate for parallel polarization considering underlying layers.
FNS	$n_s$	Refractive index of substrate.
GAM1	$\gamma_1$	See Section 3.3.
GAM2	$\gamma_2$	See Section 3.3.
RHØ	$\rho = R_{21}^p / R_{21}^n$	Ratio of reflection coefficient.
RHØ1	$\rho$	Calculated from first set of values of P and A.
RHØ2	$\rho$	Calculated from second set of values of P and A.
RHØC	$\rho_c$	Complex constant of wave plate defined by eq. 1.
RN	$r_n$	Fresnel reflection coefficient for light polarized normal to the plane of incidence.
RP	$r_p$	Fresnel reflection coefficient for light polarized parallel to the plane of incidence.

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## Appendix I

### Use of the ALINE Instruction in Relation to Alinement of the Ellipsometer

Carl Fenstermaker

This appendix describes a modification of the alinement procedure of McCrackin, et al [4]. In the procedure described below the components are not adjusted in their holders to correct errors in the readings of their associated scales. Instead, errors in the scale readings are measured and used to correct future readings. Physical adjustment to 0.01 degree of the components within their scales is frequently very difficult, requiring tedious small changes and rechecks to approach the accuracy of readability. This modified procedure is much faster and the alinement can be done to the accuracy of the scales on the first trial. Although all future readings must be corrected, this correction is easily made with the ALINE instruction.

We define P, A, and Q as the actual azimuthal position of the plane of transmission of the prisms of polarizer and analyzer and plane of the fast axis of the wave plate respectively, and  $P_s$ ,  $A_s$ , and  $Q_s$  as the corresponding scale readings. All azimuthal angles are measured positive counter-clockwise from the plane of incidence when looking into the light beam.

The corrections used on the ALINE card ( $\Delta P$ ,  $\Delta A$ , and  $\Delta Q$ ) are the values which, when added to the scale readings, give the actual positions of the plane of transmission of the polarizer and analyzer and the position of the fast axis of the wave plate, so

$$P = P_s + \Delta P \quad (31)$$

$$A = A_s + \Delta A \quad (32)$$

$$Q = Q_s + \Delta Q \quad (33)$$

As in Section 2.3 "Alinement Procedure" of reference [4], the wave plate is removed, the arms of the ellipsometer set in the straight through position, the scale reading of the polarizer,  $P_s$ , set to zero and the azimuth of the analyzer is adjusted to a value near  $90^\circ$  that gives a minimum in the transmitted light. At the minimum the polarizer and analyzer are crossed so that

$$A = P + 90^\circ,$$

or by eqs 31 and 32

$$A_s + \Delta A = \Delta P + 90^\circ$$

since  $P_s = 0$ .

Defining  $\epsilon = A_s - 90^\circ$  gives

$$\Delta A = \Delta P - \epsilon. \quad (34)$$

We record  $\epsilon$  instead of adjusting the analyzer scale to make it zero as in reference 4.

For the alinement of the polarizer, a metal surface is used with the arms set for reflection at an angle near the principal angle. The analyzer is set with the plane of transmission approximately in the plane of the surface ( $A_s \approx 90^\circ$ ). As described in reference 4, the polarizer then is adjusted for minimum transmission ( $P_s \approx 0^\circ$ ) and the intensity of the minimum noted.  $A_s$  is moved by 0.1 degree and  $P_s$  is again adjusted for a minimum and the intensity noted. If the intensity has increased  $A_s$  is adjusted in the opposite direction. By taking a series of readings, setting the analyzer by increments, and adjusting the polarizer for a minimum, we can plot  $P_s$  versus  $A_s$  and determine the point on this curve which intersects the line  $P_s = A_s - \epsilon - 90^\circ$  which is also the line  $P = A - 90^\circ$ .

We may also approach this point directly by using smaller and smaller increments of  $A_s$  in an attempt to find scale readings  $P_s$  and  $A_s$  such that

$$A_s - P_s = 90^\circ + \epsilon \quad (35)$$

within 0.01 degree. Thus, the point at which both  $P = A - 90^\circ$  and minimum transmission occur is obtained by setting  $A_s$  and adjusting  $P_s$ . This method has been shown to be the only unambiguous way of alining the ellipsometer [4]. At this point the plane of transmission of the polarizer is in the plane of incidence; therefore,  $P = 0$  and, by eq 31,  $\Delta P = -P_s$  and  $\Delta P$  is determined.  $\Delta A$  can then be calculated by eq 34.

The wave plate is alined by inserting it between crossed polarizer and analyzer in the straight through position with the polarizer set at zero ( $P = 0^\circ$ ,  $A = 90^\circ$  or  $P_s = -\Delta P$ ,  $A_s = 90^\circ - \Delta A$ ) and adjusting it near the zero reading of the fast axis for minimum transmission. At this minimum the fast axis of the wave plate will be set to the azimuth of the polarizer which is zero. By eq 33,

$$Q_s + \Delta Q = 0^\circ$$

$$\Delta Q = -Q_s \quad (36)$$

The three alinement corrections,  $\Delta P$ ,  $\Delta A$ , and  $\Delta Q$ , have now been obtained and may be used on the ALINE card as shown in table 2.



## Appendix II

### Derivation of Equation 3

The derivation uses Jones vector and matrices as described in "Polarized Light" by W. Shurcliff [15].

The normalized Jones vector of the light from the polarizer, expressed in x and y axes along the fast and slow axes of the wave plate, is  $\begin{bmatrix} \cos (P-Q) \\ \sin (P-Q) \end{bmatrix}$  where P and Q are azimuths of the polarizer and fast axis of the wave plate measured from the plane of incidence of the reflection. The matrix for the wave plate is  $\begin{bmatrix} 1 & 0 \\ 0 & \rho_c \end{bmatrix}$ .

The light is now expressed with respect to x and y axes along and normal to the plane of incidence by use of the counter-rotator matrix  $\begin{bmatrix} \cos Q & -\sin Q \\ \sin Q & \cos Q \end{bmatrix}$ .

The matrix for reflection from the surface is simply  $\begin{bmatrix} \rho & 0 \\ 0 & 1 \end{bmatrix}$ .

Therefore, the light after reflection from the surface is given by

$$\begin{bmatrix} \rho & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} \cos Q & -\sin Q \\ \sin Q & \cos Q \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & \rho_c \end{bmatrix} \begin{bmatrix} \cos (P-Q) \\ \sin (P-Q) \end{bmatrix}$$

$$= \begin{bmatrix} \rho[\cos Q \cos (P-Q) - \rho_c \sin Q \sin (P-Q)] \\ \sin Q \cos (P-Q) + \rho_c \cos Q \sin (P-Q) \end{bmatrix}.$$

For this light to be extinguished by the analyzer, it must be linearly polarized. In this case, its azimuth e is given by

$$\tan e = \frac{\sin Q \cos (P-Q) + \rho_c \cos Q \sin (P-Q)}{\rho[\cos Q \cos (P-Q) - \rho_c \sin Q \sin (P-Q)]}$$

$$= \frac{\tan Q + \rho_c \tan (P-Q)}{\rho[1 - \rho_c \tan Q \tan (P-Q)]}.$$

The analyzer must be set  $90^\circ$  from  $e$  to extinguish the light so

$$\tan A = -1/\tan e ;$$

therefore,

$$\tan A = \frac{\rho[\rho_c \tan Q \tan (P-Q) - 1]}{\tan Q + \rho_c \tan (P-Q)} \cdot$$

Solving for  $\rho$  gives eq 3.



```

NM      1.33
NF      2.5      0.3
A1      65.
CNS     86.35   25.19   176.35   154.81   45.
        86.350   25.190   176.350   154.810   45.000
DELI=   97.300003 PSI1= 25.189998 DEL2= 97.300007 PSI2= 25.190002
DEL=    97.300006 PSI= 25.189999
INDEX OF SUBSTRATE= 2.0000 DEL= 97.300 PSI= 25.190
CD      94.30   24.44   45.
        94.300   24.440   45.000
DEL=    A1.400000 PSI= 24.439999
INDEX OF MEDIUM= 1.33000 ANGLE OF INCIDENCE= 65.000 WAVE LENGTH= 5461.00 TC= 1.00000 DELC= 90.000
THICK N2 REAL KAPPA ADSORPTION Δ DEL Δ PSI ERROR N2-N1 N3=N2 WT FRACTION NS REAL KAPPA K
100.6 2.50000 .38000 4.8265=03 -.00% .023 -.38856 1.17000 -.50005 4.79826 1.99995 1.00016 2

```

Figure 2. Instructions CNS and CD.

```

A1      60.
WL      5893.
NS      1.5163
NF      1.1     .25     1.5
CND     16.943  11.856
INDEX OF MEDIUM= 1.00000 ANGLE OF INCIDENCE= 60.000 WAVE LENGTH= 5893.00 TC= 1.00000 DELC= 90.000
THICK N2 REAL KAPPA ADSORPTION Δ DEL Δ PSI ERROR N2-N1 N3=N2 WT FRACTION NS REAL KAPPA K
1000.0 1.40000 .00000 8.2425=03 =.001 =.000 .01848 .40000 .11630 .82425 1.51630 .00000 2

```

Figure 3. Instruction CND.





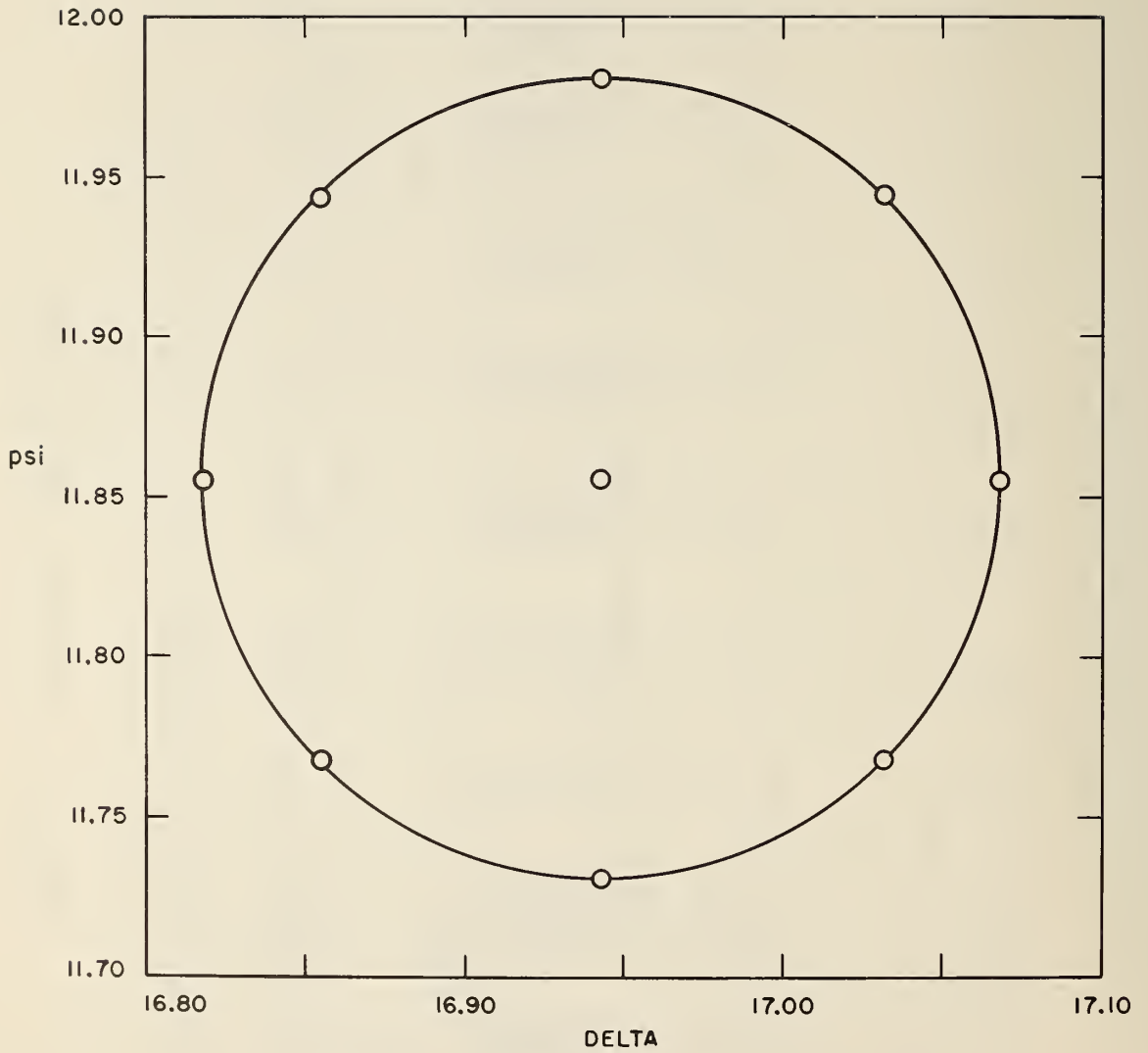


Figure 5. Confidence ellipse for measurements  $\Delta$  and  $\psi$  .

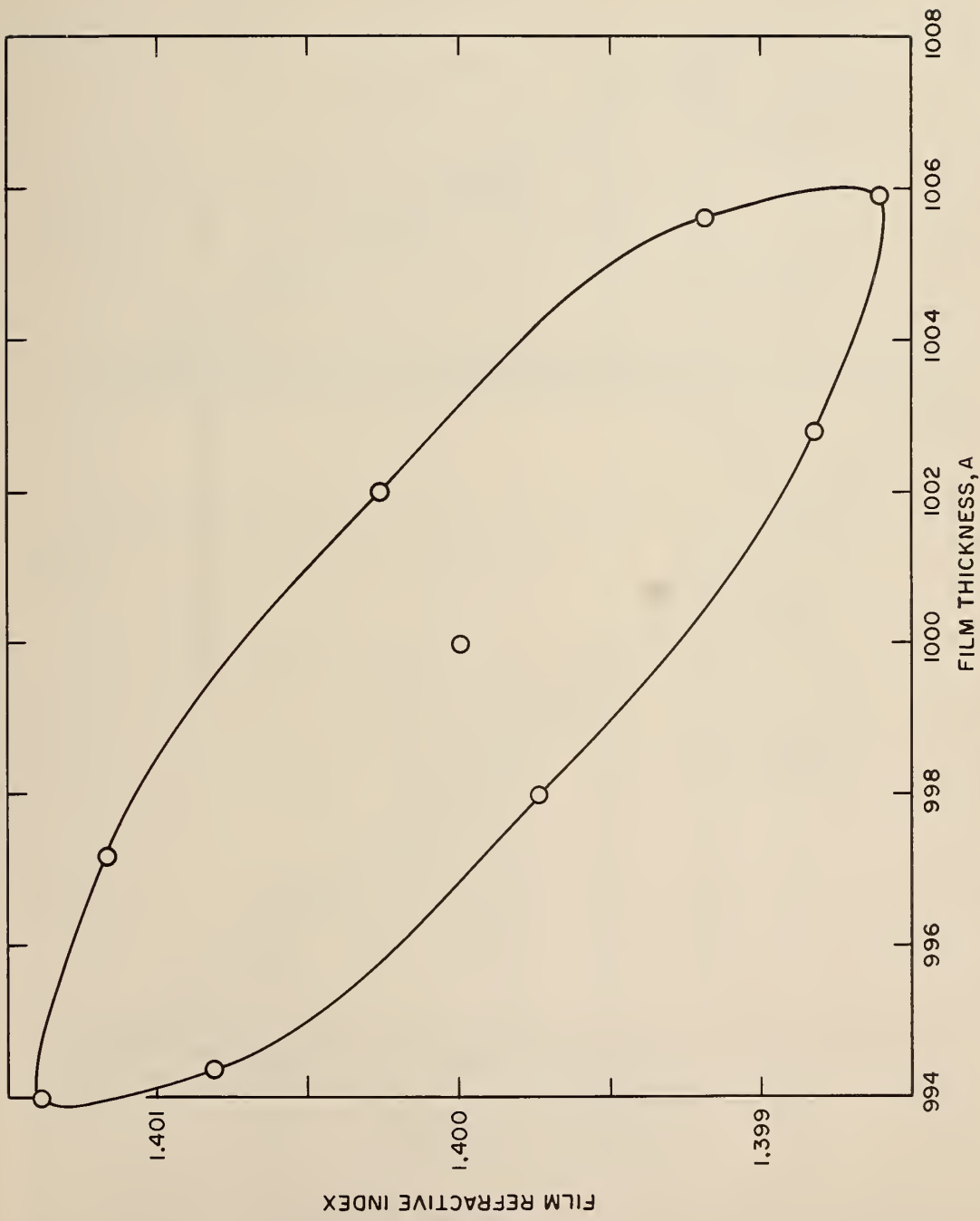
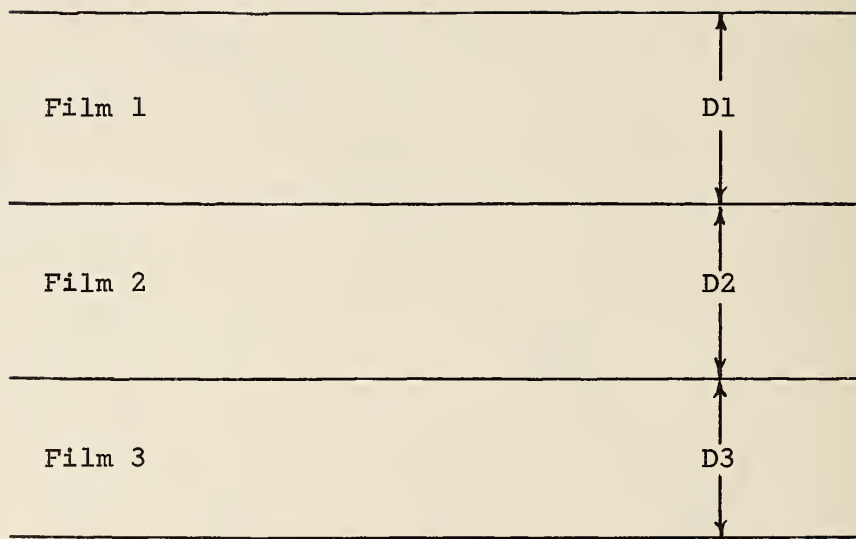


Figure 6. Confidence ellipse for calculated values of the refractive index and thickness of the film.

Surrounding  
Medium



Substrate

Fig. 7. . - Schematic diagram of three films on a Substrate.

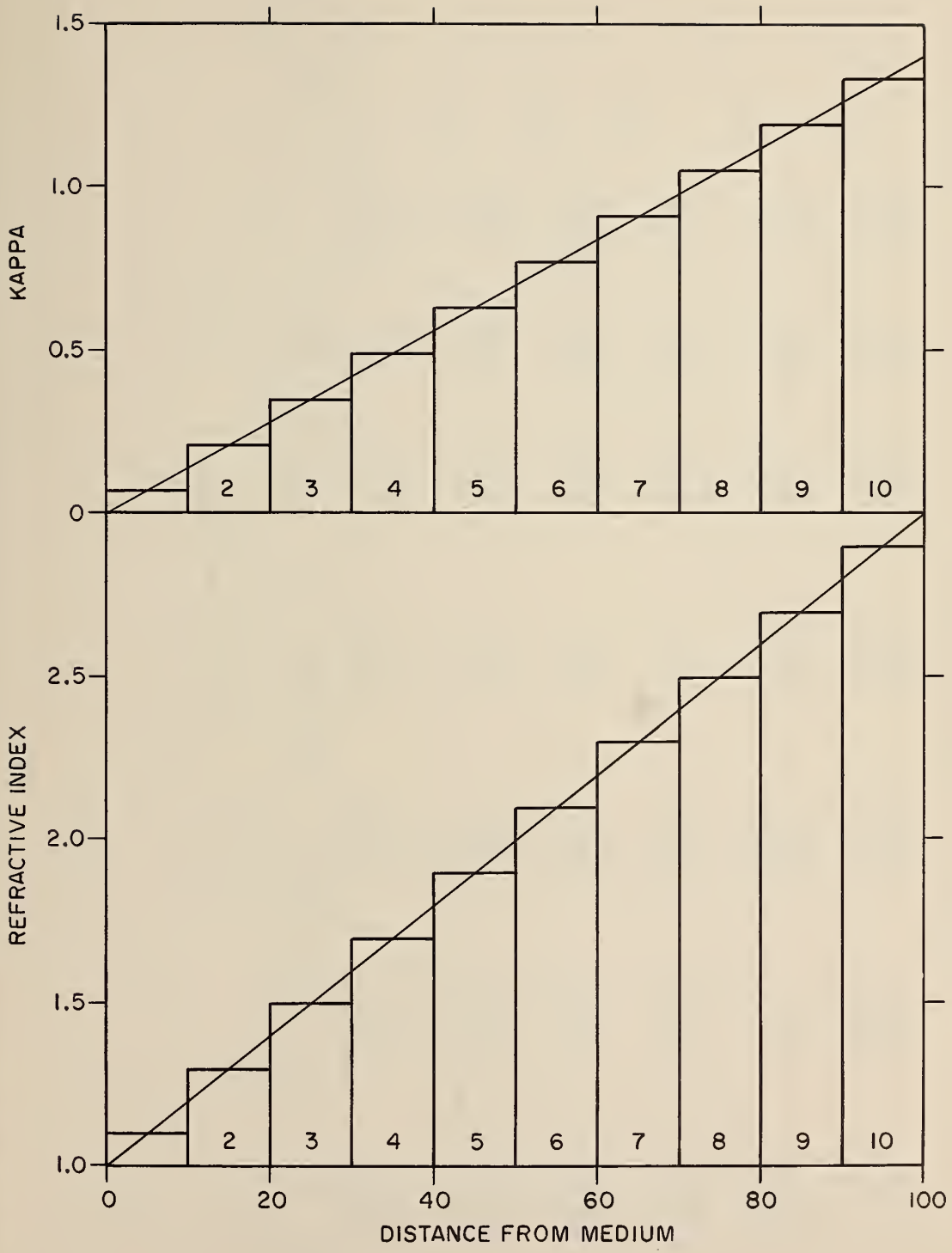


Figure 8. Approximation of an inhomogeneous film by ten homogeneous films.







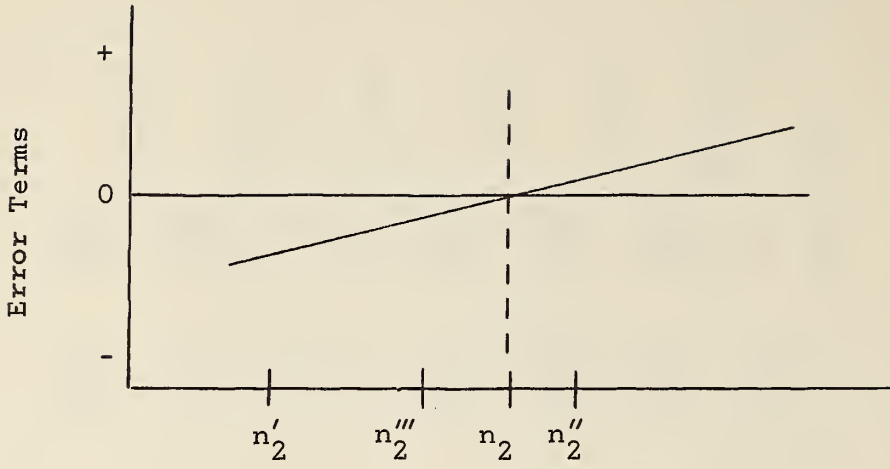


Figure 11a. Refractive index of film.

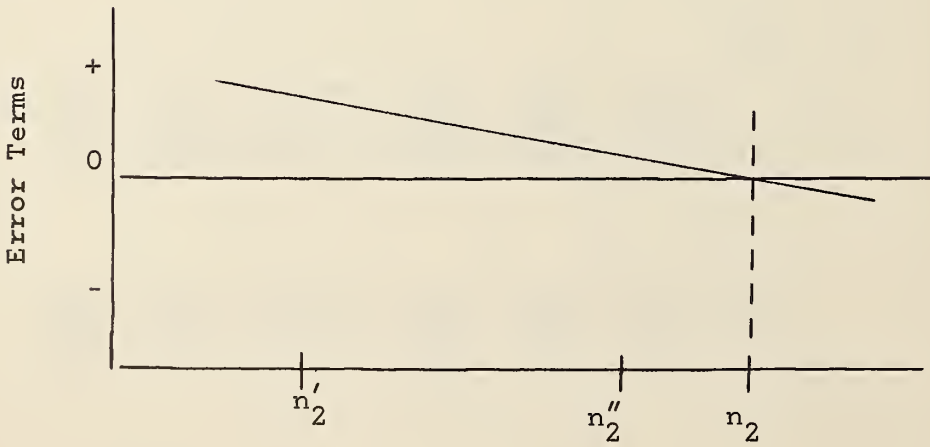


Figure 11b. Refractive index of film.

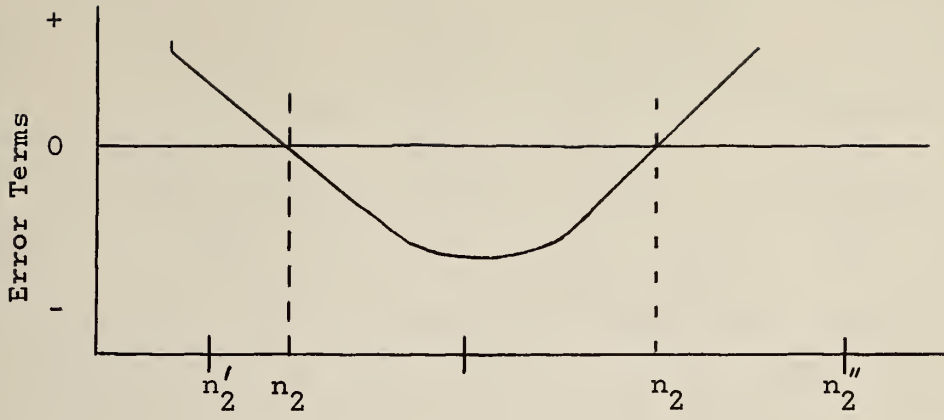


Figure 11c. Refractive index of film.

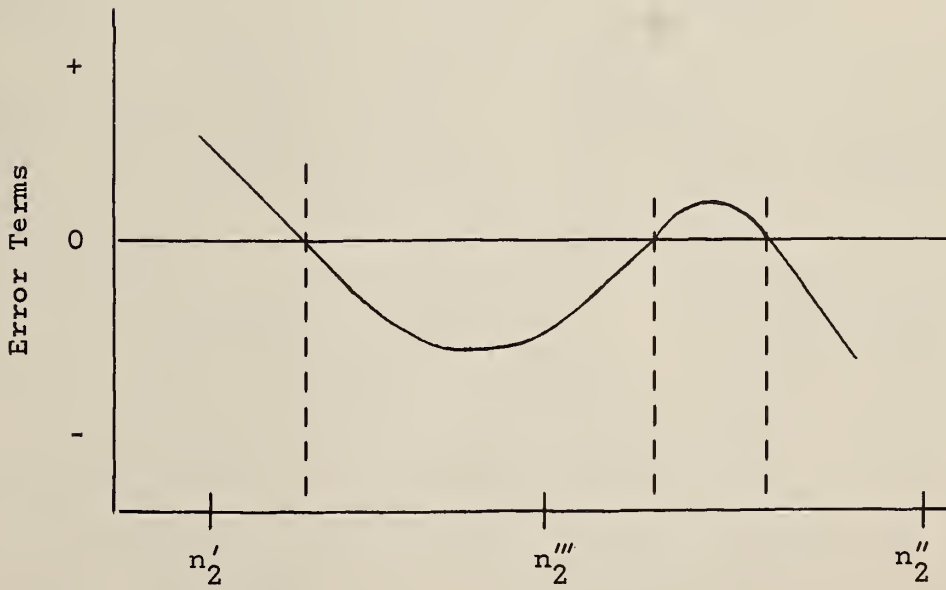


Figure 11d. Refractive index of film.





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