

Copyright © 1966, by the author(s).
All rights reserved.

Permission to make digital or hard copies of all or part of this work for personal or classroom use is granted without fee provided that copies are not made or distributed for profit or commercial advantage and that copies bear this notice and the full citation on the first page. To copy otherwise, to republish, to post on servers or to redistribute to lists, requires prior specific permission.

SOME COMPUTER PROGRAMS USEFUL IN ELLIPSOMETRY

by

W. H. Oldham

Memorandum No. ERL-M173

26 August 1966

ELECTRONICS RESEARCH LABORATORY

College of Engineering
University of California, Berkeley
94720

Manuscript submitted: 14 June 1966

The research reported herein was supported wholly by the Joint Services Electronics Program (U. S. Army, U. S. Navy, U. S. Air Force) under Grant No. AF-AFOSR-139-66.

SOME COMPUTER PROGRAMS USEFUL IN ELLIPSOMETRY

Because of the tedious and often transcendental nature of the computations necessary to reduce ellipsometric data, a series of programs have been developed. All but one are written in Fortran IV language as implemented on the Berkeley DCS (IBM 7090) system, the exception being a Quiktran program.

In ellipsometry, one measures the effect of reflection from a surface on the two components (polarizations) of an incident light beam. In particular, the ratio of the two complex reflection coefficients R_p and R_s for light polarized with the electric vector in and normal to the plane of incidence, respectively, is defined as $\tan \Psi e^{i \Delta}$. In the usual experimental scheme Ψ and Δ are essentially read directly from the instrument settings.¹ The computational task then is to relate Ψ and Δ to the properties of the reflecting object. If we model this object as consisting of a semi-infinite solid with one or more homogenous films of various (constant) thicknesses, the classical theory of optics relates Ψ and Δ to the complex indices of refraction of the substrate and films, the thicknesses of the films, and the other independent variables,

namely the angle of incidence, the index of refraction of the immersing medium (usually air), and the wavelength of light used in the measurement. Thus, there exist two equations¹

$$\Psi = f (n_s, n_{F1}, n_{F2} \dots n_{Fn}, t_{F1}, t_{F2} \dots t_{Fn}, \phi, n_1, \lambda), \quad (1)$$

$$\Delta = g (n_s, n_{F1}, n_{F2} \dots n_{Fn}, t_{F1}, t_{F2} \dots t_{Fn}, \phi, n_1, \lambda). \quad (2)$$

The essential difficulties may be stated as:

1. The functions f and g are extremely tedious to compute involving numerous operations on complex numbers (an average of 10^{-2} sec are required per computation of Ψ and Δ on the IBM 7090 computer).
2. The inverse functions f^{-1} and g^{-1} are known only for the case of a film-free substrate, thus one must either resort to iterative guessing schemes or to graphical methods in order, for example, to solve for n_{F1} and t_{F1} given the other independent variables and having measured Ψ and Δ .
3. If more than two of the independent variables are unknown, then a single measurement of Ψ and Δ is insufficient information to determine the unknowns. Obviously, several measurements at various wavelengths or angles of incidence, etc. could be made and

a self-consistent solution could be found. However, certain difficulties must be overcome:

- a. The method may be too insensitive to discriminate when using certain variables, e. g. , angle of incidence. ²
- b. Immense amounts of information must be scanned if even only three unknowns exist, e. g. , suppose one seeks the real film thickness t and the real and imaginary parts of the index of refraction $\underline{n = ik}$ of a thin film, with all other variables known. One could measure $\underline{\Psi = \Psi(\lambda)}$ and $\Delta = \Delta(\lambda)$ at various wavelengths and proceed as follows: Assume $k=0$, and plot Ψ and Δ vs t for various values of n . At the point on the Ψ, Δ plane where $\Psi = \Psi(\lambda)$ and $\Delta = \Delta(\lambda)$, we have a possible solution $k=0, t=t_0, n=n_0$. Now one repeats the process assuming $k=k_1$ which yields t_1, n_1 . Doing this many times one may plot n or t vs k . The whole process is repeated for a different wavelength, and the second plot of n or t vs k is prepared, and the intersection of the two plots would yield the correct values of n, t, k . (Other methods are possible.) ²

The above difficulties in data reduction made it necessary to prepare programs so that interesting films could be examined . Another rather complete program in existence is described by McCrackin and Colson. ² It was implemented here by R. S. Muller but proved unsatisfactory because of its failure to find a satisfactory

solution to the third problem discussed above. Rather than patch this program to our needs, T. I. Kamins and R. S. Muller wrote two programs in Fortran IV to compute and plot Δ and Ψ from Eqs. (1) and (2) for the case of a single film. These programs have since been slightly modified and only the modified versions are described here. The remaining programs were written as needed for various other tasks described. All certainly are "patched" and undoubtedly slower than optimum, but insofar as is known are completely debugged.

PROGRAMS

- Program "plot" (1) - Computes Δ and Ψ for single film on a substrate.
- Program "plot" (2) - Computes Δ and Ψ for two films on a substrate.
- Program "graph" - Computes and plots (CAL COMP PLOTTER)
 Δ and Ψ for a single film on a substrate.
- Program "index" - Computes the substrate index of refraction from a measurement of Δ and Ψ .
- Program "Pfeiff" - Quiktran program to compute substrate index of refraction from a measurement of Δ and Ψ .
- Program "Optmin" - Computes the film index of refraction by a graphical method for absorbing or non-absorbing films.

DESCRIPTION OF THE PROGRAMS (all except Pfeiff in Fortran IV)

PROGRAM "PLOT" (Jan. 17 version)

This program computes Ψ and Δ for a system consisting of a film with a complex index of refraction N_2 and thickness(es) THICK, THICK + ALPHA, THICK + 2 ALPHA . . . THICK + N ALPHA on a substrate with a complex index of refraction N_3 in an immersing medium with a complex index of refraction N_1 . The angle of incidence is PHI_{II} and the wavelength $LAMBDA$. As may be seen from the listing, the computation is divided into three parts:

- i. a section that prints headings, reads data cards, and defines the number of computations (N)
- ii. a subroutine that computes the interfacial reflection coefficients, and
- iii. a subroutine that computes and prints Ψ and Δ .

The INPUT DATA should be in the form of:

PHI_{II} (11 - 20)

$LAMBDA$ (11 - 20)

N_1 (11 - 20 real, 21 - 30 imag.)

N_3 (11 - 20 real, 21 - 30 imag.)

N_2 (11 - 20 real, 21 - 30 imag.), $THICK$ (41 - 50), $ALPHA$ (61 - 70),

N (76 - 80)

N2 THICK, ALPHA, N

. " " "

. " " "

. " " "

N2 " " "

BLANK

PHI11

LAMBDA

etc.

The program reads another N2 card after a complete set of Ψ and Δ for the various thicknesses is computed and proceeds to compute another complete set for each N2 card. After a blank card, the program expects to find a complete new data set starting with PHI11. The program halts by running into a \$EOF card, i. e., it runs out of data. The DATA FORMAT is all real F10.0 except N which is integral; thus, decimals and signs (imaginary parts of the indices of refraction are zero or negative) must be put in for the real data.

The computation speed is about 10 ms/computation, i. e., the running time is approximately $0.01 \times N$ sec per N2 card. A sample output is given in Table 1. Binary and source decks are available.

PROGRAM "GRAPH" (May 8 version)

This program is essentially the same as "plot" above except

ANGLE OF INCIDENCE (PHI11) = 70.00 DEGREES
 WAVE LENGTH (LAMBDA) = 6328. ANGSTROMS
 INDEX OF REFRACTION OF IMMERSING MEDIUM (N1) = 1.0000 0.0000
 INDEX OF REFRACTION OF THIN FILM (N2) = 1.2000 -0.0000
 INDEX OF REFRACTION OF SUBSTRATE (N3) = 3.8500 -0.3000
 INITIAL THICKNESS = 0. ANGSTROMS
 THICKNESS INCREMENT (ALPHA) = 10. ANGSTROMS
 NUMBER OF INCREMENTS (N) = 400

THICKNESS (ANGSTROMS)	CHANGE IN PHASE WHILE TRAVERSING FILM (SMALL DELTA-DEGREES)	PSI (DEGREES)	DELTA (DEGREES)
0.	0.00	10.69	167.78
10.	0.42	10.74	166.09
20.	0.85	10.79	164.42
30.	1.27	10.86	162.76
40.	1.70	10.93	161.12
50.	2.12	11.01	159.51
60.	2.55	11.10	157.92
70.	2.97	11.19	156.35
80.	3.40	11.28	154.81
90.	3.82	11.39	153.30
100.	4.25	11.50	151.82
110.	4.67	11.61	150.36
120.	5.09	11.73	148.93
130.	5.52	11.86	147.53
140.	5.94	11.99	146.16
150.	6.37	12.13	144.82
160.	6.79	12.27	143.51
170.	7.22	12.41	142.23
180.	7.64	12.56	140.98
190.	8.07	12.71	139.76
200.	8.49	12.87	138.57
210.	8.92	13.03	137.40
220.	9.34	13.19	136.27
230.	9.77	13.35	135.16
240.	10.19	13.52	134.08
250.	10.61	13.70	133.03
260.	11.04	13.87	132.00
270.	11.46	14.05	131.00
280.	11.89	14.22	130.02
290.	12.31	14.41	129.07
300.	12.74	14.59	128.14
310.	13.16	14.77	127.24
320.	13.59	14.96	126.36
330.	14.01	15.15	125.50
340.	14.44	15.34	124.67
350.	14.86	15.53	123.85
360.	15.28	15.72	123.06
370.	15.71	15.92	122.29
380.	16.13	16.11	121.53
390.	16.56	16.31	120.80

Table 1.

that the results (Δ and Ψ for various thicknesses) are manipulated in a third subroutine and put onto a tape for Calcomp plotting. A plot is produced in the Ψ - Δ plane with thickness as a running parameter along the curve. Several options are available:

1. The program will automatically choose its own scale, or alternatively the limits on the coordinates may be specified MINPSI, MAXPSI, MIN DEL, and MAX DEL.

2. A grid may be plotted (automatically scaled) or suppressed. When the value of 1 for NOGRID is encountered, the grid is suppressed.

3. One or more curves may be plotted on the same graph (frame). When a value of 1 for NXTFRM is encountered in the data, the plotter moves one frame.

4. An "x" is marked on the curve every NTH thickness value, i. e., at thickness = THICK, thickness = THICK + N x NTH x ALPHA, etc.

The INPUT DATA should be in the following form:

NTH (6 - 10), MINPSI (16 - 20), MAXPSI (26 - 30), MINDEL (36 - 40),

MAXDEL (46 - 50), NXTFRM (56 - 60), NOGRID (66 - 70) (all integers)

PHI 11 (as in "plot")

LAMBDA "

N1 "

N3 "

N2, THICK, ALPHA, N (as in "plot")

N2

.
.
.

N2

BLANK (ONE, TWO, OR THREE BLANKS)

NTH

PHI 11

etc.

ONE BLANK card has the effect of causing the entire data set (NTH, PHI 11 . . . N2) to be reread and another set of curves (according to how many values of N2) to be plotted with the same coordinates, scale, and grid, on the same frame; the NXTFRM option on the first card should be zero.

TWO BLANK cards have the effect of causing the entire data set to be reread and the grid recomputed -- usually then the NXTFRM option on the first card would be one.

THREE BLANK cards have the effect of halting the program.

The computation speed is approximately the same as "plot", i. e., about 10^{-2} sec per point. A sample output is given in Table 2 and Fig. 1. Binary and source decks are available.

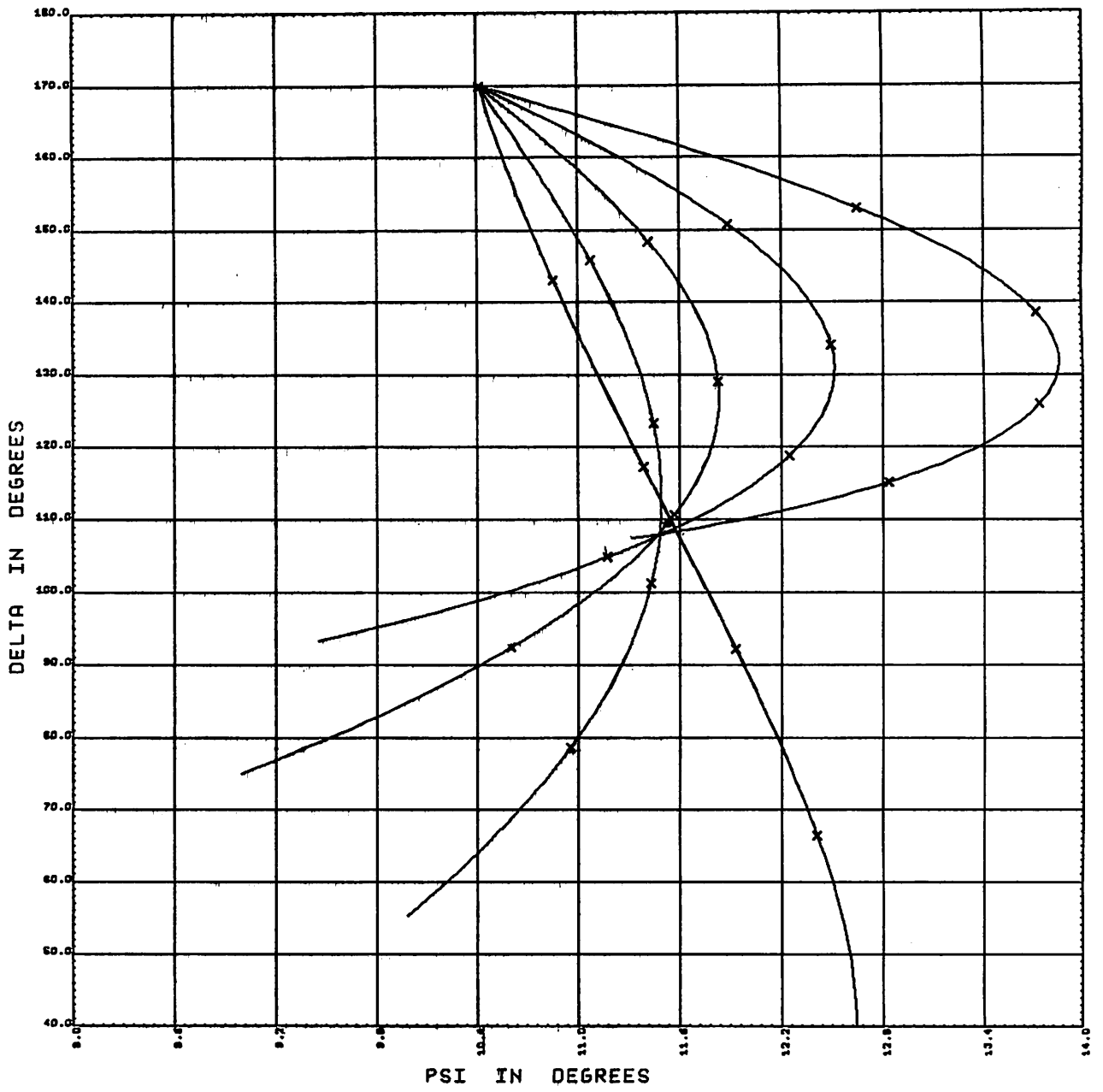


Fig. 1.

ANGLE OF INCIDENCE (PHI11) = 70.00 DEGREES

WAVE LENGTH (LAMBDA) = 6328. ANGSTROMS

INDEX OF REFRACTION OF IMMERSING MEDIUM (N1) = 1.0000 0.0000

INDEX OF REFRACTION OF THIN FILM (N2) = 2.7000 -0.0944

INDEX OF REFRACTION OF SUBSTRATE (N3) = 3.8300 -0.2400

INITIAL THICKNESS = 6328. ANGSTROMS

THICKNESS INCREMENT (ALPHA) = 5. ANGSTROMS

NUMBER OF INCREMENTS (N) = 100

CHANGE IN PHASE			
THICKNESS (ANGSTROMS)	WHILE TRAVERSING FILM (SMALL DELTA-DEGREES)	PSI (DEGREES)	DELTA (DEGREES)
0.	0.00	10.42	169.91
5.	0.72	10.44	168.53
10.	1.44	10.46	167.15
15.	2.16	10.48	165.78
20.	2.88	10.50	164.41
25.	3.60	10.52	163.04
30.	4.32	10.54	161.68
35.	5.04	10.56	160.32
40.	5.76	10.58	158.96
45.	6.48	10.60	157.61
50.	7.20	10.62	156.26
55.	7.92	10.64	154.92
60.	8.64	10.67	153.57
65.	9.36	10.69	152.24
70.	10.08	10.71	150.90
75.	10.80	10.74	149.57
80.	11.52	10.76	148.24
85.	12.24	10.79	146.92
90.	12.96	10.81	145.60
95.	13.68	10.84	144.28
100.	14.40	10.86	142.97
105.	15.12	10.89	141.66
110.	15.84	10.91	140.35
115.	16.56	10.94	139.05
120.	17.28	10.96	137.74
125.	18.00	10.99	136.45
130.	18.72	11.02	135.15
135.	19.44	11.04	133.86
140.	20.16	11.07	132.57
145.	20.88	11.09	131.28
150.	21.60	11.12	129.99
155.	22.32	11.15	128.71
160.	23.04	11.18	127.43
165.	23.76	11.20	126.15
170.	24.48	11.23	124.87
175.	25.20	11.26	123.60
180.	25.92	11.28	122.33
185.	26.64	11.31	121.06
190.	27.36	11.34	119.79
195.	28.08	11.37	118.52

Table 2.

PROGRAM "PLOT (2)" (Mar. 7 version)

This program is also a variation on "PLOT"; it computes Ψ and Δ for a system consisting of two films and a substrate. All parameters are as in plot except that the bottom film complex index of refraction is N4 and thickness is T4. N2 is the complex index of refraction of the top film and its thickness is incremented as in "PLOT."

The INPUT DATA should be in the following form:

PHI11 (as in "plot")
LAMBDA "
N1 "
N3 "
N4 (11-20, 21-30), Tr (31-40) (F10,0 format - use decimals
and signs)
N2 (as in "plot")
N2 "
. . .
N2
BLANK
PHI11
LAMBDA
etc.

A blank card has the effect of causing the program to reread an entire new data set.

The computation speed is the same as "plot." A sample output is given in Table 3. Binary and source decks are available.

PROGRAM "INDEX" (Feb. 20)

This program computes the substrate index refraction from the measured values of Δ and Ψ on film-free sample.

The INPUT DATA are on one card in the form of PSI (11-20), DELTA (31-40), PHI (51-60) (all are real and should include a decimal.)

The computation will be made for as many data cards as are in the deck. A sample output is given in Table 4.

PROGRAM "PFEIFF" (Jan. 21)

This is a QUIKTRAN program which computes the substrate index of refraction from the measured values of Δ and Ψ for a film-free sample.

To use the program, one first gets the QUIKTRAN console in COMMAND mode (indicated by a - READY reply) then types (TAB)* LOAD (PFEIFF) and upon receiving a + READY reply, may initiate execution by typing (TAB) START (0), at which point the computer will request data.

* (TAB) means hit the TAB key.

BOTT LAYER INDEX= 2.50000 -2.10000
 AND THICKNESS= 122.0000
 ANGLE OF INCIDENCE (PHI1) = 70.00 DEGREES
 WAVE LENGTH (LAMBDA) = 6328. ANGSTROMS
 INDEX OF REFRACTION OF IMMERSING MEDIUM (N1) = 1.0000 0.0000
 INDEX OF REFRACTION OF THIN FILM (N2) = 1.6000 0.0000
 INDEX OF REFRACTION OF SUBSTRATE (N3) = 3.7860 -0.4372
 INITIAL THICKNESS = 0. ANGSTROMS
 THICKNESS INCREMENT (ALPHA) = 10. ANGSTROMS
 NUMBER OF INCREMENTS (N) = 60

 122. 36.72 170.54

THICKNESS (ANGSTROMS)	CHANGE IN PHASE WHILE TRAVERSING FILM (SMALL DELTA-DEGREES)	PSI (DEGREES)	DELTA (DEGREES)
0.		18.83	137.29
10.		19.04	135.35
20.		19.26	133.45
30.		19.49	131.59
40.		19.73	129.77
50.		19.97	127.99
60.		20.22	126.25
70.		20.47	124.55
80.		20.72	122.89
90.		20.98	121.27
100.		21.25	119.69
110.		21.51	118.14
120.		21.78	116.63
130.		22.05	115.15
140.		22.33	113.71
150.		22.60	112.30
160.		22.88	110.92
170.		23.16	109.58
180.		23.43	108.27
190.		23.71	106.99
200.		23.99	105.74
210.		24.28	104.52
220.		24.56	103.32
230.		24.84	102.16
240.		25.12	101.02
250.		25.40	99.91
260.		25.68	98.83
270.		25.96	97.77
280.		26.25	96.74
290.		26.53	95.73
300.		26.81	94.75
310.		27.09	93.79
320.		27.37	92.85
330.		27.65	91.94
340.		27.93	91.05
350.		28.21	90.18
360.		28.49	89.33

Table 3.

PSI = 41.50000
DELTA = 133.04000
ANGLE OF INC = 70.00000
THE SUBSTRATE INDEX OF REFRACTION IS 0.98805 +J -5.73166

PSI = -0.00000
DELTA = -0.00000
ANGLE OF INC = -0.00000
THE SUBSTRATE INDEX OF REFRACTION IS -0.00000 +J 0.00000

FXEM CALLED. ERROR TYPE = 059
END OF INPUT DATA
JOB TERMINATED.

ERROR TRACE. CALLS IN REVERSE ORDER.
CALLING ROUTINE LINE NO. ABSOLUTE LOCATION
F103 203 14134
FRDD 50 15461
INDEX 1 3101
END OF TRACE

ERROR EXIT XR1= 63643 XR2= 00001 XR4= 67267 XR3= 00001 XR5= 00000 XR6= 00000 XR7= 00000
END EXECUTION 13JOB BCDCS 00026.16

Table 4.

The INPUT DATA are typed in format (TAB) PSI/DELTA/PHI; all should include decimals. A sample output is shown in Table 5.

PROGRAM "OPTIMIN" (Mar. 23 version)

This program is an attempt to attack data-handling problem (3) mentioned above. Assuming one knows the substrate index of refraction and either (a) the real part of the film index, or (b) the imaginary part of the film index, one computes from the measured Δ and Ψ values the thickness and (a) the imaginary film index or (b) the real film index. In practice, one has neither situation (a) nor (b) thus one computes a number of sets $n_1, k_1, t_1; n_2, k_2, t_2; \dots$ which satisfy the measurements. The "correct" set may be found by using additional information, e. g., an independent measurement on a film of a different thickness.

The method of solution is essentially graphical and may best be described by an example. Suppose one has measured the values Δ_0 and Ψ_0 and wishes to assume that the imaginary part of the film index is zero. Furthermore, one believes that the real film index n_f lies between 1.0 and 4.0. The program computes the $\Delta - \Psi$ plot vs thickness (a curve on the $\Delta - \Psi$ plane) for each of $n_f = 1.0, n_f = 1.0 + \alpha, n_f = 1.0 + 2\alpha, \dots, n_f = 4.0$, where α is chosen by the user. It then decides both which curve comes closest to Δ_0, Ψ_0 , and what point on this curve is closest, i. e., the real part of the index n_f and

```

;USER(BE3306)
FULL QUIKTRAN SERVICE AVAILABLE
001  READY
;CONSOLE
101. -READY
LOAD(PFEIFF)
129. +READY
START(0)
107. =0 02
107. = 2
107. = 3
107. = 4
107. = 5 TAB AND ENTER PSI DELTA PHI IN DECIMAL DEGREE IN FORMAT X./Y./Z.
108. =0 03 PSI DELTA PHI
109. =1 00 11.1/161./70.
126. =0 99
126. = 2
126. = 3 RESULTS ARE N K NK
127. =0 00 3.83405 0.12501 0.47930
107. =0 02
107. = 2
107. = 3
107. = 4
107. = 5 TAB AND ENTER PSI DELTA PHI IN DECIMAL DEGREE IN FORMAT X./Y./Z.
108. =0 03 PSI DELTA PHI
109. =1 00 11.1/170./70.
126. =0 99
126. = 2
126. = 3 RESULTS ARE N K NK
127. =0 00 3.92071 0.06681 0.26195
107. =0 02
107. = 2
107. = 3
107. = 4
107. = 5 TAB AND ENTER PSI DELTA PHI IN DECIMAL DEGREE IN FORMAT X./Y./Z.
108. =0 03 PSI DELTA PHI
109. =1 00 11.1/172. 70.
126. =0 99
126. = 2
126. = 3 RESULTS ARE N K NK
127. =0 00 3.93308 0.05356 0.21067
107. =0 02
107. = 2
107. = 3
107. = 4

```

Table 5.

the thickness t_f . It then reduces the area searched on the $\Delta - \Psi$ plane by reducing the range of thickness and the index searched by a factor of two and continues the search on a finer scale. It will do this as many times as desired.

Thus, in practice, one selects:

- (a) The range of thickness values to be examined,
- (b) The increments of thickness (i. e., the "distance" between data points for a given curve on a $\Delta - \Psi$ "plot"),
- (c) The value of either (i) the real part of the film index of refraction or (ii) the imaginary part of the film index of refraction, and correspondingly,
- (d) The range of either (i) the imaginary index or (ii) the real index,
- (e) The increments in either the (i) imaginary index or (ii) the real index, i. e., the "distance" between "curves" on the $\Delta - \Psi$ "plot,"
- (f) The reduction factor for the thickness increments on the second and following pass,
- (h) The number of passes, and
- (i) The printout options (to be described).

The actual method of selection of the best index and thickness involves the comparison of Δ_0 , Ψ_0 with discrete points (and lines drawn between them) on the Δ , Ψ plane. Thus, the thickness

increments must not be too large or the program will not see the curvature in the $\Delta - \Psi$ locus and fail to converge.

The INPUT DATA should be arranged as follows:

PHI 11 (11-20), LAMBDA (31-40)

N1 (11-20, 21-30), N3 (41-50, 51-60)

PSI 0 (11-20), DELTA 0 (31-40)

THICK (11-20), D THICK (13-40), F THICK (51-60)

P1 (11-15), P2 (16-20), P3 (21-25), P4 (26-30), P5 (31-35)

N2 (11-20, 21-30), FN2R (31-40), FN2I (41-50), DN2R (51-55),

DN2I (56-60), DT (61-65), DN (66-70), L (71-72)

N2 etc.

.
..
.

N2 etc.

BLANK

PHI 11

etc.

PHI 11 is the angle of incidence (decimal degrees).

LAMBDA is the wavelength (real, include decimal).

N1 is the index of refraction of the immersing medium (complex, include sign and decimal).

N3 is the index of refraction of the substrate (complex, include sign and decimal).

PSIO and DELTAO are the measured Ψ and Δ values (decimal degrees).

THICK and F THICK are the beginning and end of the thickness range, and

D THICK is the thickness increment (all are real, include the decimal).

P1 is a debug print option and should be left blank.

P2 controls the printing of the individual Δ , Ψ values for each thickness; if P2 = 1 (integer) a list of Δ and Ψ vs thickness is produced as in program "plot"; if P2 = 0, this listing is not made. The value of the error, i. e., the distance to the Δ_0 , Ψ_0 point, is also printed.

P3 is a debug printing option and is normally left blank.

P4 controls the printing of the output array. See sample output, Table 6. If P4 is 0, the array is printed; a 1 (integer) will suppress it.

P5 controls the printing of nearby output arrays, i. e., the next nearest values of the film index to the optimum. A zero calls for the printout; a 1 suppresses it. One notes that the usual situation is all zeros for P1 - P5, except occasionally when one wants everything printed and therefore opts P2 = 1, all others are zero. (Thus a blank card will suffice for this card.)

N2 specifies the initial value of N2 (complex, includes decimals and signs).

300.00	13.15	116.17	9.65
350.00	12.87	109.88	2.08
400.00	12.38	101.91	6.98
450.00	11.71	95.29	12.93
500.00	10.84	89.13	19.70

THE VALUES OF THE PARAMETERS AT THE OPTIMUM -- MINUS ONE INCREMENT VALUE OF N2			
FOR THE FILM INDEX OF THICKNESS	2.90000 PSI	-0.90000 DELTA	THE OPTIMUM THICKNESS IS 450.00 ERROR
350.00	15.18	115.00	10.50
400.00	14.84	109.65	4.82
450.00	14.30	104.85	5.96
500.00	13.61	100.69	9.42
550.00	12.78	97.32	11.96

THE VALUES OF THE PARAMETERS AT THE OPTIMUM -- PLUS ONE INCREMENT VALUE OF N2			
FOR THE FILM INDEX OF THICKNESS	2.90000 PSI	-0.30000 DELTA	THE OPTIMUM THICKNESS IS 300.00 ERROR
200.00	11.40	127.24	19.32
250.00	11.29	117.16	9.37
300.00	11.02	107.07	1.58
350.00	10.59	96.82	12.26
400.00	10.00	86.28	23.40

HERE WE GO AGAIN WITH A SMALLER MESH

****THE VALUES OF THE PARAMETERS AT THE OPTIMUM VALUE OF N2 ARE TABLED HERE****

ANGLE OF INCIDENCE =	70.		
WAVELENGTH =	6328.		
AIR INDEX =	1.00000 0.00000		
SUBSTRATE INDEX =	3.84100 -0.26000		
THE VALUES OF THE PARAMETERS AT THE OPTIMUM -- MINUS ONE INCREMENT VALUE OF N2			
FOR THE FILM INDEX OF THICKNESS	2.90000 PSI	-0.45000 DELTA	THE OPTIMUM THICKNESS IS 333.33 ERROR
300.00	12.07	112.41	4.80
316.67	11.97	109.57	1.86
333.33	11.84	106.74	1.61
350.00	11.70	103.93	4.28
366.67	11.54	101.13	7.00

THE VALUES OF THE PARAMETERS AT THE OPTIMUM -- MINUS ONE INCREMENT VALUE OF N2			
FOR THE FILM INDEX OF THICKNESS	2.90000 PSI	-0.55000 DELTA	THE OPTIMUM THICKNESS IS 350.00 ERROR
316.67	12.71	112.48	5.52
333.33	12.60	109.84	2.87
350.00	12.48	107.42	1.56
366.67	12.33	104.93	3.91
383.33	12.16	102.47	6.20

THE VALUES OF THE PARAMETERS AT THE OPTIMUM -- PLUS ONE INCREMENT VALUE OF N2			
FOR THE FILM INDEX OF THICKNESS	2.90000 PSI	-0.35000 DELTA	THE OPTIMUM THICKNESS IS 333.33 ERROR
300.00	11.36	109.06	1.19
316.67	11.24	105.88	2.55
333.33	11.11	102.69	5.88
350.00	10.95	99.48	9.24
366.67	10.77	96.27	12.63

HERE WE GO AGAIN WITH A SMALLER MESH

Table 6.

FN2R specifies the maximum value of the real part of N2 to be tried and DN2R the increments in the real part of N2.

FN2I and DN2I are similar; normally however only one is varied, e. g. , FN2R = Real (N2) and DN2R = 0 or FN2I = Imag (N2) and DN2I = 0. (All are real and should include decimals and signs).

DT and DN specify the reduction factor for the thickness and index increment, respectively, (real, include decimal).

L specifies the number of passes (integer).

Obviously, the fastest procedure in such a search is a binary choice, however it almost certainly would not converge. A satisfactory compromise found here is to use ten thickness and ten index increments, i. e. , 100 computations per pass. Then the increments are reduced by 2 or 3 each time, and 4 or 5 passes are made. Thus, if THICK = 0; D THICK = 100 ; F THICK = 1000, N2 = 2.0 - j2.0, FN2R = 2.0, DN2R = 0.0, FN2I = 0; DN2I = 0.2, DT = 2.0, DN = 2.0, L = 5, we will determine the index to within 0.012 and the thickness to within 6. in 500 computations.

The computation speed is about 8ms/point or 4 sec for the above example.

The computations will be made for as many N2 cards as are in a sequence. A blank card will cause the computer to read a complete data set PHI 11 ... etc. , and two blanks will halt the program.

A sample output is shown in Table 6. Binary and source decks are available.

REFERENCES

1. For a description of the instrument and the method of measurement

see:

F. L. McCrackin, E. Passaglia, R. R. Stromberg, and

H. L. Steinberg. J. Research NBS A67, 363 1963.

2. F. L. McCrackin and S. P. Colson in "Ellipsometry in the

Measurement of Surfaces and Thin Films" NBS Misc Pub

w56, 1963.