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COMPUTER PROGRAMS FOR ELLIPSOMETRY

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COMPUTER PROGRAMS FOR ELLIPSOMETRY

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ABSTRACT

This report gives a collection of computer programs in FORTRAN IV language which are used in ellipsometry. Two programs (programs CMER and CMOC) can be used to determine optical parameters of bare surfaces. The correction of the deviation of the compensator from ideal retardation and transmission has been incorporated in the computation of optical constants of bare surfaces derived from measurements in one zone (program OZOM). Two other programs permit the use of ellipsometer azimuth readings as input and output variables to determine the refractive index and film thickness of a film-covered surface (programs FILM and A3PLOT). This is of advantage in case of comparison of calculated and measured polarizer- and analyzer-readings which are recorded from an automatic ellipsometer. Another program converts ellipsometer azimuth readings into relative phase and amplitude parameter (Δ, ψ) (program PSIDEL).

I. Introduction

In ellipsometry, the change of the state of polarization due to reflection is measured and interpreted in terms of properties of the reflecting surface. This technique is capable of examining surfaces in any optically transparent environment. The reflection of light from surfaces and thin films has been discussed by various authors.[2-4]

Two parameters are measured in ellipsometry: the change in relative amplitude (ψ) and relative phase (Δ) of two orthogonal quantities of light due to reflection. From these two measured quantities two parameters of the reflecting surface can be derived. For a bare surface, this can be the real and imaginary part of the complex refractive index. For a surface covered with a transparent film, the real refractive index of the dielectric film and the thickness can be determined, if the optical constants of the substrate are known. Sometimes it is possible to determine more than two unknowns, i.e., thickness and complex refractive index of an absorbing film, if sufficiently narrow limits can be given for the unknowns.

The exact classical equations[10] cannot be solved explicitly[11] and are too tedious for normal calculations in all but a few cases. The availability of high-speed computers therefore is an important factor in ellipsometry. Such programs given below can be used with ellipsometers either manually or automatically operated.

The first two programs (CMER and CMOC) can be used to determine optical parameters of bare surfaces from ellipsometer readings and vice versa. The deviation of the compensator from ideal retardation and transmission has been considered in program OZOM. The next two programs (FILM and A3PLOT) allow to compare calculated with measured azimuth readings of the ellipsometer of film covered surfaces. For the application of an automatic ellispometer, which records the azimuth readings of analyzer and polarizer, it is very convenient to compare calculated and measured azimuth readings. In the case of manual operation, program SPIDEL can be used to convert ellispometer azimuth readings into relative phase and amplitude parameters (Δ, ψ)

All formulas derived below are based on the Nebraska convention.[12]

II. FORTRAN IV Computer Program "CMER"

This program computes the ellipsometeric parameters Δ and ψ * from given values of the complex refractive index n_c of bare surfaces using the complex formalism.** Application of the electromagnetic theory[3,4] shows that the Fresnel equations can be adopted to describe reflection from absorbing media by introduction of a complex refractive index n_c:

$$n_c = n - ik \quad . \tag{1}$$

n_c is defined here to be a material constant, independent of angle of incidence.[5,6] Application of Snell's law

$$n_o \sin\phi = n_c \sin\phi_c' \tag{2}$$

results in a complex angle of refraction ϕ_c', which provides a valid formalism, but no recognisable physical meaning. (n_o real refractive index of incident medium, ϕ angle of incidence). The Fresnel equations[7] relate the amplitude of reflection coefficients to the angles of incidence and refraction.

$$r_p = \frac{\tan(\phi - \phi_c')}{\tan(\phi + \phi_c')} \tag{3}$$

$$r_s = -\frac{\sin(\phi - \phi_c')}{\sin(\phi + \phi_c')} \tag{4}$$

*Derivation of Δ and ψ from ellipsometer azimuth of analyzer, polarizer and quarter-wave plate can be found in Table I.

**A previous program "MER"[1], which avoided the complex formalizm[2] and was based on earlier work,[13] leads to the same results.

Using trigonometric formulas, one gets

$$\cos(\phi + \phi_c') = \cos\phi \cos\phi_c' - \sin\phi \sin\phi_c' \tag{5}$$

$$\cos(\phi - \phi_c') = \cos\phi \cos\phi_c' + \sin\phi \sin\phi_c' \tag{6}$$

$$\sin(\phi + \phi_c') = \sin\phi \cos\phi_c' + \cos\phi \sin\phi_c' \tag{7}$$

$$\sin(\phi - \phi_c') = \sin\phi \cos\phi_c' - \cos\phi \sin\phi_c' \tag{8}$$

where $\sin\phi_c'$ and $\cos\phi_c'$ are given by applying Eq. (2)

$$\sin\phi_c' = (n_o \sin\phi)/n_c \tag{9}$$

$$\cos\phi_c' = \sqrt{1 - \sin\phi_c'^2} = \sqrt{\frac{n_c^2 - n_o^2 \sin^2\phi}{n_c^2}} \tag{10}$$

The Fresnel coefficients represent the ratio of reflected to incident electric field amplitude and are different for s and p components[4]

$$r_p = \left|\frac{E_p''}{E_p}\right| e^{i(\varepsilon_p'' - \varepsilon_p)} = \frac{E_p''}{E_p} \tag{11}$$

$$r_s = \left|\frac{E_s''}{E_s}\right| e^{i(\varepsilon_s'' - \varepsilon_s)} = \frac{E_s''}{E_s} \tag{12}$$

with the modulus representing the amplitude attenuation

$$|r_p| = \left|\frac{E_p''}{E_p}\right| \tag{13}$$

$$|r_s| = \left|\frac{E_s''}{E_s}\right| \tag{14}$$

and the argument representing the (absolute) change in phase due to reflection

$$\delta_p = \varepsilon''_p - \varepsilon_p \tag{15}$$

$$\delta_s = \varepsilon''_s - \varepsilon_s \tag{16}$$

Thus, the complex Fresnel reflection coefficients can also be expressed as

$$r_p = |r_p| \; e^{i\delta_p} \tag{17}$$

$$r_s = |r_s| \; e^{i\delta_s} \tag{18}$$

The ellipsometer determines the ratio ρ of the (complex) reflection coefficients for p and s components

$$\rho = \frac{r_p}{r_s} = \left|\frac{r_p}{r_s}\right| e^{i(\delta_p - \delta_s)} \tag{19}$$

which is often given in a simplified form as

$$\rho = \tan\psi \; e^{i\Delta} \tag{20}$$

Comparison with Eq. (19) leads to the definitions

$$\tan\psi = \left|\frac{r_p}{r_s}\right| \tag{21}$$

$$\Delta = \delta_p - \delta_s \tag{22}$$

The absolute change in phase due to reflection then is expressed by

$$\delta_p = \tan^{-1} \frac{\mathrm{Im}(r_p)}{\mathrm{Re}(r_p)} \tag{23}$$

$$\delta_s = \tan^{-1} \frac{\mathrm{Im}(r_s)}{\mathrm{Re}(r_s)} \tag{24}$$

The ellipsometric parameters Δ and ψ can be computed from Eq. (19) to give

$$\Delta = \tan^{-1} \frac{\mathrm{Im}(\rho)}{\mathrm{Re}(\rho)} \tag{25}$$

$$\psi = \tan^{-1} (|\rho|) \tag{26}$$

Variables Employed in CMER Program

Name	Symbol	Description
TNO	n_o	Refractive index of transparent incident medium
TNC	n_c=n-ik	Complex refractive index of metal
PHID	ϕ(deg)	Angle of incidence
PHI	ϕ(rad)	Angle of incidence
DELD	Δ(deg)	Rel. phase change $\delta_p - \delta_s$
PSID	ψ(deg)	$\tan^{-1}$ of rel. amplitude attenuation
RHO	ρ	Ratio of reflexion coefficients of p- and s-component: r_p/r_s
RHO REAL	Re(ρ)	Real part of ρ
RHO IMAG	Im(ρ)	Imaginary part of ρ
RPC	r_p	Reflection coeff. of p-component (complex)
RSC	r_s	Reflection coeff. of s-component (complex)
RP	$\|r_p\|$	Modulus of r_p
RS	$\|r_s\|$	Modulus or r_s
DELPD	δ_p	Absolute phase change with respect to incident wave (p-component)
DELSD	δ_s	Absolute phase change with respect to incident wave (s-component)
ABSRHO	$\|\rho\|$	Modulus of ρ

Input Data for the Program "CMER"

The input data are punched on cards as illustrated below:

Card	Col. 1-10	Col. 11-20
1	TITLE	(Col. 1-80)
2	ϕ(deg)	n_o
3	n	-k

Cards 1-3 constitute one set. Three blank cards must follow the last set of data. The program together with a sample output is given below.

CMER

```
                PROGRAM CMER (INPUT,OUTPUT)
          C     THIS PROGRAM IS INDEPENDENT OF ANGLE READINGS
          C     THIS PROGRAM COMPUTES THE PARAMETERS FOR METALLIC
          C     REFLECTION FROM VALUES OF TNC,TNO AND PHID USING COMPLEX NUMBER
          C
                COMPLEX RHO,TNC,S2,S3,S4,C2,C3,C4,RPC,RSC
          C
                DIMENSION TITLE (8)
              5 READ 76,TITLE
   10         1 READ 10,PHID,TNO
             10 FORMAT (2F10.0)
             76 FORMAT (8A10)
   20           PRINT 77,TITLE
             77 FORMAT (1H0,8A10)
   26         2 READ 20,TNC
             20 FORMAT (2F10.0)
   34           IF (TNC) 12,12,4
   37         4 CONTINUE
          C
   37         3 PRINT 30,PHID,TNC,TNO
             30 FORMAT (1H0,7HPHID = ,F10.7,/, 6HTNC = ,F10.7,F10.7,/,6HTNO = ,
               1F10.7,/)
               2,8X,2HRP,10X,5HDELPD,7X,2HRS,10X,5HDELSD)
          C
   51           ALPHA=0.01745329252
   52           PHI=PHID*ALPHA
   54           S1 = SIN (PHI)
   56           C1 = COS (PHI)
   60           S2 = (TNO*S1)/TNC
   72           C2 = CSQRT (1 - S2*S2)
  111           C3 = (C1*C2)+(S1*S2)
  123           C4 = (C1*C2)-(S1*S2)
  135           S3=S1*C2-C1*S2
  147           S4=S1*C2+C1*S2
          C
  162           RPC=(S3*C4)/(C3*S4)
  205           RSC=-S3/S4
  215           RHO=RPC/RSC
          C
  224           ABSRHO=CABS(RHO)
  226           PSID=ATAN(ABSRHO)/ALPHA
  231           DELD=ATAN2(AIMAG(RHO),REAL(RHO))/ALPHA
  240           RP=CABS(RPC)
  242           RS=CABS(RSC)
  244           DELPD=ATAN2(AIMAG(RPC),REAL(RPC))/ALPHA
  253           DELSD=ATAN2(AIMAG(RSC),REAL(RSC))/ALPHA
  262           IF (DELPD.LT.0.0) DELPD = DELPD + 360
  266           IF (DELSD.LT.0.0) DELSD=DELSD + 360.
  271           IF (DELD.LT.0.0) DELD=DELD + 360.
          C
  274           PRINT 80,RHO,ABSRHO,RP,RS,DELPD,DELSD,PSID,DELD
             80 FORMAT (1H0,6HRHO = ,2F10.5,/,9HABSRHO = ,F10.5,
               C/,5HRP = ,F10.5,10X,5HRS = ,F10.5,/,8HDELPD = ,F10.5,
               C10X,8HDELSD = ,F10.5,/,7HPSID = ,F10.5,10X,7HDELD = ,
               CF10.5,//)
  320           GO TO 5
  321        12 CONTINUE
  322           END
```

Sample Output, Program CMER

```
CU        *** CMER  ***              WAVELENGTH = 546.1 NM

 PHID = 75.0000000
TNC =    .9300000-2.3900000
TNO =  1.0000000


 RHO =      .21477    .69411
ABSRHO =       .72658
RP =       .68342            RS =       .94061
DELPD =   242.42742            DELSD =   169.62031
PSID =    36.00128            DELD =    72.80712


 AG

 PHID = 75.0000000
TNC =    .0820000-3.6100000
TNO =  1.0000000


 RHO =     -.03543    .97840
ABSRHO =       .97904
 P =       .97618            RS =       .99708
DELPD =   264.15372            DELSD =   172.07960
PSID =    44.39322            DELD =    92.07412


 AU

 PHID = 75.0000000
TNC =    .3700000-2.3500000
TNO =  1.0000000


 RHO =      .29254    .83065
ABSRHO =       .88066
RP =       .85737            RS =       .97355
DELPD =   239.15379            DELSD =   168.55504
PSID =    41.36907            DELD =    70.59876


 AL

 PHID = 75.0000000
TNC =    .8100000-5.4700000
TNO =  1.0000000


 RHO =     -.36791    .79721
ABSRHO =       .87801
RP =       .86658            RS =       .98699
DELPD =   289.54345            DELSD =   174.77036
```

```
PSID =    41.28331              DELD =  114.77209


 CR

 PHID = 75.0000000
TNC =  2.9600000-3.4500000
TND =  1.0000000


 RHO =      -.14320     .46518
ABSRHO =         .48672
RP =        .45298           RS =       .93069
DELPD =   282.08206            DELSD =   174.97189
PSID =    25.95302            DELD =   107.11018


 NI

 PHID = 75.0000000
TNC =  1.4000000-2.5200000
TND =  1.0000000


 RHO =       .13240     .61114
ABSRHO =         .62532
RP =        .57886           RS =       .92569
DELPD =   248.85213           DELSD =  171.07568
`SID =    32.01860           DELD =    77.77645


 PT

 PHID = 75.0000000
TNC =  2.8600000-4.4200000
TND =  1.0000000


 RHO =      -.24625     .52789
ABSRHO =         .58250
RP =        .55314           RS =       .94960
DELPD =   290.26584           DELSD =   175.25765
PSID =    30.22084          DELD =   115.00819


 TA

 PHID = 75.0000000
TNC =  3.5000000-2.4000000
TND =  1.0000000


  RHO =      -.08503     .32134
 ABSRHO =       .33240
 RP =        .30086           RS =       .90511
 DELPD =   280.68405           DELSD =   175.86241
 PSID =    18.38686           DELD =   104.82163
```

III. FORTRAN IV Computer Program "CMOC"

This computer program (Complex Metal Optical Constants) calculates the optical constants from relative phase change, Δ, and arctangent of relative amplitude attenuation, ψ, using the complex formalism.* This program just is the inversion of program "CMER". The ratio ρ of the (complex) reflection coefficients for p and s components can be determined from given values of Δ and ψ

$$\rho = \frac{r_p}{r_s} = \tan\psi \cdot e^{i\Delta} \tag{27}$$

Application of Fresnel's equations, Eqs. (3) and (4)

$$r_p = \frac{\tan(\phi - \phi_c')}{\tan(\phi + \phi_c')} = \frac{\frac{\sin(\phi - \phi_c')}{\cos(\phi - \phi_c')}}{\frac{\sin(\phi + \phi_c')}{\cos(\phi + \phi_c')}} \tag{28}$$

$$r_s = -\frac{\sin(\phi - \phi_c')}{\sin(\phi + \phi_c')} \tag{29}$$

leads to

$$\rho = -\frac{\cos(\phi + \phi_c')}{\cos(\phi - \phi_c')} \tag{30}$$

Use of Eqs. (5) through (8) give

$$\cos\phi_c' = \frac{\cos(\phi + \phi_c') + \cos(\phi - \phi_c')}{2\cos\phi} \tag{31}$$

and

$$\sin\phi_c' = \frac{\cos(\phi - \phi_c') - \cos(\phi + \phi_c')}{2\sin\phi} \tag{32}$$

*A previous program "MOC"[1] which avoided the complex formalism [2] and was based on earlier work,[13] leads to the same results.

$$\tan\phi_c' = \frac{1+\rho}{1-\rho}\cdot\frac{1}{\tan\phi} \tag{33}$$

$\tan\phi_c'$ can be converted to $\sin\phi_c'$ with

$$\sin\phi_c' = \frac{\tan\phi_c'}{\sqrt{1+\tan^2\phi_c'}} \tag{34}$$

Then the (complex) refractive index is determined by

$$n_c = n - ik = \frac{n_o \sin\phi}{\sin\phi_c'} \tag{35}$$

Variables Used in Program "CMOC"

Name	Symbol	Description
PHID	ϕ(deg)	Angle of incidence
PHI	ϕ(rad)	Angle of incidence
DELD	Δ(deg)	Rel. phase change
DEL	Δ(rad)	Rel. phase change
PSID	ψ(deg)	Arctangent of rel. amplitude attenuation
PSI	ψ(rad)	Arctangent of rel. amplitude attenuation
TNO	n_o	Refractive index of incident medium (dielectricum)
TNC	n_c	Refractive index of metal (complex)
TN	n	$Re(n_c)$
TK	k	$Im(n_c)$

Input Data for Program "CMOC"

The input data for the program CMOC are arranged on cards as illustrated below.

Card	Col. 1-10	Col. 11-20
1	TITLE	(Col. 1-80)
2	n_o	ϕ(deg)
3	ψ(deg)	Δ(deg)

Cards 1-3 constitute one set. Three blank cards must follow the last set of data. The program together with a sample output is given below.

CMOC

```
      PROGRAM CMOC (INPUT,OUTPUT)
C     THIS PROGRAM IS INDEPENDENT OF ANGLE READINGS
C     THIS PROGRAM COMPUTES N AND K FOR METALLIC REFLECTION
C     FROM VALUES OF DELD,PSID,PHID AND TNO USING COMPLEX NU8BERS
C
      COMPLEX RHO,T2,S2,TNC,I
      DIMENSION TITLE (8)
    1 READ 76,TITLE
      READ 3,TNO,PHID
    3 FORMAT (2F10.0)
   76 FORMAT (8A10)
      PRINT 77,TITLE
   77 FORMAT (1H0,8A10)
      READ 3,PSID,DELD
      IF (PSID) 100,100,2
    2 PRINT 4
    4 FORMAT (4HPHID,9X,3HTNO,8X,4HPSID,7X,4HDELD,10X,2HTN,10X,2HTK)
      ALPHA=0.01745329252
      PHI=PHID*ALPHA
      PSI=PSID*ALPHA
      DEL=DELD*ALPHA
      I=CMPLX (0.0,1.0)
      RHO=TAN(PSI)*CEXP(I*DEL)
      S1=SIN(PHI)
      T1=TAN(PHI)
      T2=(1.0 + RHO)/((1.0 - RHO)*T1)
      S2=T2/CSQRT(1.0 + T2*T2)
      TNC=(TNO*S1)/S2
C
      TN=REAL(TNC)
      TK=AIMAG(TNC)
      PRINT 6,PHID,TNO,PSID,DELD,TN,TK
    6 FORMAT (F10.7,5F12.7)
      GO TO 1
  100 CONTINUE
      END
```

```
 AL        ***  CMOC  ***
PHID          TNO         PSID         DELD            TN           TK
75.0000000    1.0000000   41.2830000  114.7730000     .8100655    -5.4699769
```

IV. FORTRAN IV Computer Program "OZOM"

This program (One Zone Measurement) calculates the optical constants from ellipsometer readings of one zone taking into consideration the error introduced by the quarter wave plate.

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 phase retardation, Δ_c, along the axes giving ρ_c.

This claculation is based on the formulas given by McCrackin.[8]

All angles are measured positive counterclockwise from the plane of incidence. The components of the ellipsometer must be arranged in the order of light source, polarizer, quarter wave plate, reflecting surface, analyzer and light detector.

The value of ρ_c is calculated from readings of the polarizer and analyzer of two zones for one Q-value (quarter-wave circle reading), i.e., a two-zone measurement, (zone 1+3 or 2+4) which gives the angle-readings of the polarizer (P_1,P_2) and of the analyzer (A_1, A_2), is necessary to compute the error of the quarter-wave plate.* Note that the one-zone-measurement has to be carried out with the same Q-value as the two-zone measurement.

Let P_i, A_i($i = 1,2$) and Q be angles of two polarizer, analyzer and quarter-wave plate-settings, respectively, for extinction of the light. The quarter-wave plate is characterized by

*Table I defines different zones.

$$\rho_c = T_c \exp(+i\Delta_c) \tag{36}$$

where T_c is the ratio of the transmittance along its fast axis to the transmittance along its slow axis:

$$T_c = \frac{1}{\sqrt{-\tan(P_1 - Q)\tan(P_2 - Q)}} \tag{37}$$

and the phase retardation Δ_c along the axes

$$\tan\Delta_c = \frac{-B^2 - \tan(P_1 - Q\tan(P_2 - Q)}{B} \tag{38}$$

where B is determined by

$$B = \frac{\tan A_1[\tan(P_2 - Q)\tan Q - \tan(P_1 - Q)/\tan Q]}{2(\tan Q_1 - \tan A_2)} - \frac{\tan A_2[\tan(P_1 - Q)\tan Q - \tan(P_2 - Q)/\tan Q]}{2(\tan A_1 - \tan A_2)} \tag{39}$$

The surface is characterized by the complex value ρ (Eq. (19))

$$\rho = \frac{r_p}{r_s} = \frac{|r_p|}{|r_s|} e^{i(\delta_p - \delta_s)} \tag{40}$$

The value of ρ is to be calculated from azimuth of P, A, Q.[9]

$$\rho = \frac{\tan A[\tan Q \mp \rho_c \tan(P - Q)]}{\rho_c \tan Q \tan(P - Q) - 1} \tag{40}$$

Having computed ρ, formulas of program "CMOC": are used: Application of Fresnel's Eqs. (28) and (29)

$$r_p = \frac{\tan(\phi - \phi_c')}{\tan(\phi + \phi_c')} = \frac{\dfrac{\sin(\phi - \phi_c')}{\cos(\phi - \phi_c')}}{\dfrac{\sin(\phi + \phi_c')}{\cos(\phi + \phi_c')}} \tag{28}$$

$$r_s = -\frac{\sin(\phi - \phi_c')}{\sin(\phi + \phi_c')} \tag{29}$$

leads to

$$\rho = -\frac{\cos(\phi + \phi_c')}{\cos(\phi - \phi_c')} \tag{30}$$

Use of Eqs. (5) through (8) give

$$\cos\phi_c' = \frac{\cos(\phi + \phi_c') + \cos(\phi - \phi_c')}{2\cos\phi} \tag{31}$$

$$\cos\phi_c' = \frac{\cos(\phi - \phi_c') - \cos(\phi + \phi_c')}{2\sin\phi} \tag{32}$$

which leads to

$$\tan\phi_c' = \frac{1 + \rho}{1 - \rho}\ \frac{1}{\tan\phi} \tag{33}$$

$\tan\phi_c'$ can be converted to $\sin\phi_c'$ with

$$\sin\phi_c' = \frac{\tan\phi_c'}{\sqrt{1 + \tan^2\phi_c'}} \tag{34}$$

Then the (complex) refractive index is determined by

$$n_c = n - ik = \frac{n_o \sin\phi}{\sin\phi_c'} \tag{35}$$

Variables Used in This Program

Name	Symbol	Description
TC	T_c	Ratio of transmittance along the fast axis to the transmittance along its slow axis of compensator
DELC	Δ_c	Phase retardance along the fast axis minus the phase retardance along the slow axis of compensator
RHOC	ρ_c	Complex number, characterizing the quarter-wave plate
RHO	ρ	Ratio of Reflection coefficients of p- and s-component (complex)
DELD	Δ	Phase of (ρ)
PSID	ψ	Modulus of (ρ)
TNO	n_o	Refractive index of transparent incidence medium
TNC	n_c	Refractive index of reflecting surface (complex)
TN	n	$Re(n_c)$
TK	k	$Im(n_c)$
PD1	P_1(deg)	Azimuth of P(Zone 1(2)) of the two-zone measurement
PD2	P_2(deg)	Azimuth of P(Zone 3(4)) of the two-zone measurement
AD1	A_1(deg)	Azimuth of A(Zone 1(2)) of the two-zone measurement
AD2	A_2(deg)	Azimuth of A(Zone 3(4)) of the two-zone measurement
QD	Q(deg)	Azimuth of Q (compensator)
AD	A	A-azimuth of a one-zone measurement (Zone 1 or 3 (2 or 4)) (deg)
PD	P	P-azimuth of a one-zone measurement (Zone 1 or 3 (2 or 4)) (deg)
PHID	ϕ	Angle of incidence
WL	λ_o	Vacuum wavelength (Angstroms)

Input Format for Program "OZOM"

Card	1-10	11-20	21-30	31-40	41-50
1, 2	TITLE and Comments				
3	n_o	ϕ	λ_o		
4	P_1	P_2	A_1	A_2	Q
5	P	A			

Cards 1-5 constitute one set. Three blank cards must follow the last set of data. All input data of angles should be in degrees. The program together with a sample output is given below.

OZOM

```
            PROGRAM OZOM (INPUT,OUTPUT)
     C      THIS PROGRAM USES AZIMUTH READINGS
     C      THIS PROGRAM COMPUTES N AND K FOR METALLIC REFLECTION
     C      USING EXPERIMENTAL VALUES FROM ONE ZONE
     C
            COMPLEX RHO,T2,S2,TNC,I,RHOC
            DIMENSION TITLE (8), RANGE (8)
            ALPHA=0.01745329252
   3        I=CMPLX (0.0,-1.0)
   6      1 READ 76, TITLE,RANGE
         76 FORMAT (8A10/8A10)
  16        PRINT 77 , TITLE,RANGE
         77 FORMAT (1H1, 8A10//8A10)
  26        READ 3,TNO,PHID,WL
          3 FORMAT (3F10.0)
  40        IF (TNO) 100,100,4
  42      4 CONTINUE
  42        READ 81,PD1,PD2,AD1,AD2,QD
         81 FORMAT (5F10.0)
  60        READ 85,PD,AD
         85 FORMAT (2F10.0)
  70        P1=PD1*ALPHA
  72        P2=PD2*ALPHA
  73        A1=AD1*ALPHA
  75        A2=AD2*ALPHA
  76        Q=QD*ALPHA
 100        A=AD*ALPHA
 101        P=PD*ALPHA
     C
 103        B=(TAN(A1)*(TAN(P2-Q)*TAN(Q)-TAN(P1-Q)/TAN(Q))-TAN(A2)*(TAN(P1
           CTAN(Q)-TAN(P2-Q)/TAN(Q)))/2.0/(TAN(A1)-TAN(A2))
 135        DELC=ATAN2(SQRT(-B*B-TAN(P1-Q)*TAN(P2-Q)),B)
 155        TC=1.0/SQRT(-TAN(P1-Q)*TAN(P2-Q))
 172        RHOC=TC*CEXP(+I*DELC)
     C
 207        RHO  =(TAN(A)*(TAN(Q)+RHOC *TAN(P-Q)))/(RHOC *TAN(Q)*TAN(P-Q)-
 250        PSID=ATAN(CABS(RHO ))/ALPHA
 254        DELD=ATAN2(AIMAG(RHO ),REAL(RHO ))/ALPHA
 263        PHI=PHID*ALPHA
     C
 265        S1=SIN(PHI)
 267        T1=TAN(PHI)
 271        T2=(1.0 + RHO)/((1.0 - RHO)*T1)
 315        S2=T2/CSQRT(1.0 + T2*T2)
 336        TNC=(TNO*S1)/S2
 347        TN=REAL(TNC)
 350        TK=AIMAG(TNC)
 352        DELC=DELC/ALPHA
     C
 353        PRINT 10, PHID,TNO,WL
         10 FORMAT (1H0,/7HPHID = ,F5.2,10X,7HTNO =  ,F7.3,10X,13HWAVELENG
           C ,F5.0,10H ANGSTROM //)
 365        PRINT 11,PD1,AD1,PD2,AD2,QD
         11 FORMAT (1H0,/ 6HPD1 = ,F6.2,10X,7HAD1 =  ,F6.2,//,6HPD2 = ,F6.
           C10X,7HAD2 =  ,F6.2,//,6HQD =  ,F6.2)
 403        PRINT 8,TC,DELC
          8 FORMAT (1H0,/6HTC =  ,F8.4,8X,7HDELC = ,F8.4//)
```

```
      PRINT 12,PD,AD
   12 FORMAT(1H0,/6HPD =  ,F6.2,10X,7HAD =   ,F6.2//)
      PRINT 13,PSID,DELD,TN,TK
   13 FORMAT (1H0,/6HPSID =,F8.4,8X,7HDELD = ,F8.4,//,6HTN =  ,F8.4,
     C 8X,7HTK =    ,F8.4)
C
      GO TO 1
  100 CONTINUE
      END
```

Sample output, program OZOM

```
MGF2 ON CR  (3.48)        *** OZOM  ***
ZONE A3 (A1/A3)

PHID = 75.00            TNO  =    1.000          WAVELENGTH =  5461 ANGSTROM


PD1 =   18.87           AD1  =  142.47
PD2 = 108.71            AD2  =   38.42
QD  =   45.00

TC  =     1.0037        DELC =  91.1642


PD  =  108.71           AD   =   38.42


PSID = 37.9756          DELD =  52.4131
TN  =      .6438        TK   =  -1.4867
```

V. FORTRAN IV Computer Program "FILM"

This program finds the thickness and (complex) refractive index of a single film (absorbing or non-absorbing) on any substrate (absorbing or non-absorbing).* It does so by systematically combining all prescribed values of film thickness L and refractive index $n_f - ik_f$ and calculating the polarizer- and analyzer-azimuths (P_c, A_c), for each combination. Wherever a particular combination of L, n_f and k_f yields agreement with the experimentally determined readings of polarizer P_m and analyzer A_m within a specified error ε_P and ε_A, this combination appears in the output as a solution.

The formalism assumes a planar substrate covered with a planar-parallel, homogeneous, isotropic film (Fig. 1). Drude's basic equation[10]

$$\rho = \frac{(r_{1p} + r_{2p}e^{-iD})\ (1 + r_{1s}r_{2s}e^{-iD})}{(r_{1s} + r_{2s}e^{-iD})\ (1 + r_{1p}r_{2p}e^{-iD})} = \tan\psi\ e^{i\Delta} \tag{36}$$

can be solved to give calculated values of Δ and ψ by use of the following equations:**

$$r_{1s} = \frac{E_{1s}}{E_s} = \frac{n_o \cos\phi - n_{cf} \cos\phi_{cf}}{n_o \cos\phi + n_{cf} \cos\phi_{cf}} \tag{37}$$

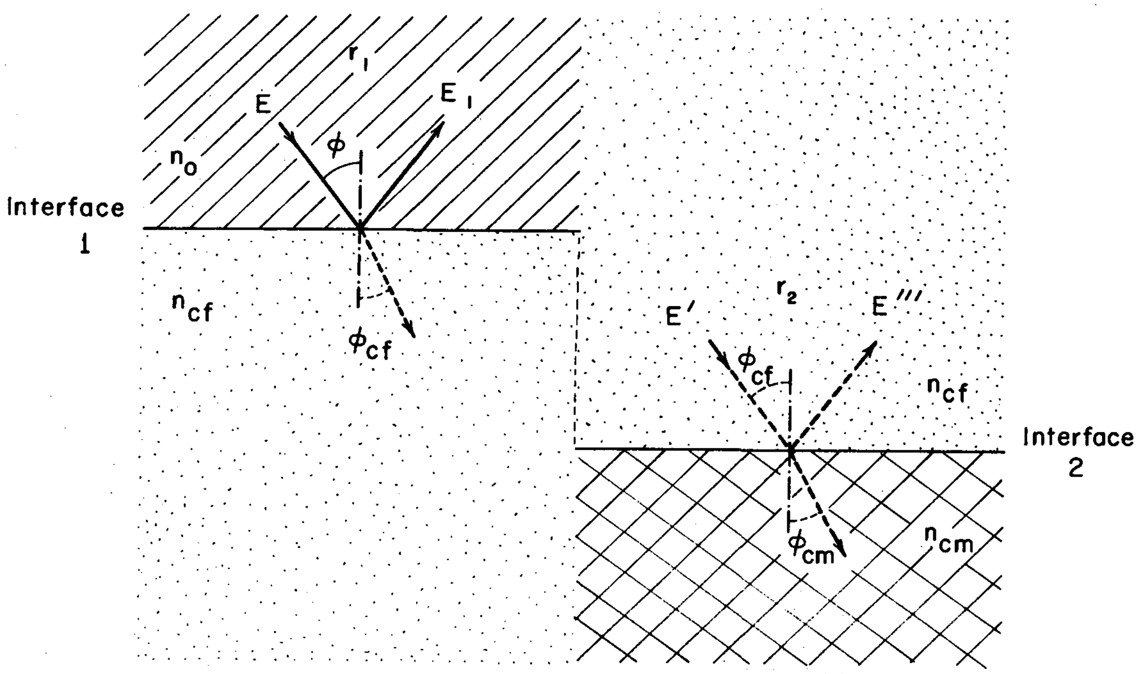
$$r_{1p} = \frac{E_{1p}}{E_p} = \frac{n_{cf} \cos\phi - n_o \cos\phi_{cf}}{n_{cf} \cos\phi + n_o \cos\phi_{cf}} \tag{38}$$

$$r_{2s} = \frac{E'''}{E'_s} = \frac{n_{cf} \cos\phi_{cf} - n_{cm} \cos\phi_{cm}}{n_{cf} \cos\phi_{cf} + n_{cm} \cos\phi_{cm}} \tag{39}$$

$$r_{2p} = \frac{E'''_p}{E'_p} = \frac{n_{cm} \cos\phi_{cf} - n_{cf} \cos\phi_{cm}}{n_{cm} \cos\phi_{cf} + n_{cf} \cos\phi_{cm}} \tag{40}$$

*Program "LAYER" (Chapter VIII) is similar to this program.

**See Fig. 1.



XBL719-4365

Fig. 1. Reflection coefficient r_1 and r_2 at both interfaces of a film-covered surface. Designation of refractive indices and electric fields. All the angles of propagation except ϕ are complex (indicated by dotted circles and lines) and cannot be interpreted geometrically.

with

$$\cos\phi_{cf} = \sqrt{1 - \frac{n_o^2 \sin^2\phi}{n_{cf}^2}} \tag{41}$$

$$\cos\phi_{cm} = \sqrt{1 - \frac{n_{cf}^2 \sin^2\phi_{cf}}{n_{cm}^2}} \tag{42}$$

and

$$D = \frac{4\pi L}{\lambda_o} n_{cf} \cos\phi_{cf} \tag{43}$$

Δ and ψ (defined in Eqs. (21) and (22)) are given by:

$$\Delta = \tan^{-1} \frac{\mathrm{Im}(\rho)}{\mathrm{Re}(\rho)} \tag{44}$$

$$\psi = \tan^{-1} (|\rho|) \tag{45}$$

The calculated polarizer and analyzer azimuths P_c and A_c are obtained according to Table I.

$$P_c = (270 - \Delta)/2$$
$$A_c = \psi$$

This program is valid for zone A-3:

range of polarizer transmission azimuth	90-135°
range of analyzer transmission azimuth	0-90°
compensator circle realing	45°

Using different zones, one has to change the conversion from P_c, A_c, Q to Δ and ψ according to Table I.

Variables Used in Program FILM

a. Real Quantities

Name	Symbol	Description
AC	A_c	Calculated azimuth angle of analyzer (deg)
AM	A_m	Measured azimuth angle of analyzer (deg)
DELC	Δ(calculated)	Relative phase change (deg)
DTN	δn_f	Iteration increment of film refractive index n_f
DTNK	δk_f	Iteration increment of index of extinction of film
DT	δL	Iteration increment of film thickness L
EAM	ε_A	Specified experimental error of A (deg)
EPM	ε_P	Specified experimental error of P (deg)
PHI1	ϕ(degrees)	Angle of incidence
PHI	ϕ(radians)	Angle of incidence
PC	P_c	Calculated azimuth angle of polarizer (deg)
PM	P_m	Measured azimuth angle of polarizer (deg)
PSIC	ψ(calculated)	Arctangent of relative amplitude attenuation (deg)
Q	Q	Measured azimuth angle of compensation (deg)
TN1	n_o	Refractive index of incident medium
TNS	n_m	Refractive index of substrate
TNKS	k_m	Index of extinction of substrate
TNI	n_{fi}	Lower limit of interaction span of film index n_f
TN	n_f	Refractive index of film
TNM	n_{fm}	Upper limit of iteration span of film index n_f
TNKI	k_{fi}	Lower limit of iteration span of k_f of film
TNK	k_f	Index of extinction of film
TNKM	k_{fm}	Upper limit of iteration span of k_f of film

Name	Symbol	Description
TI	L_i	Lower limit of iteration span for film thickness L
T	L	Film thickness (units as for λ_o)
TM	L_m	Upper limit of iteration span of film thickness
WL	λ_o	Vacuum wavelength (Angstroms)

b. Complex Qualities

Name	Symbol	Description
CPHI2	$\cos\phi'$	Complex cosine of complex angle of refraction in film
CPHI3	$\cos\phi'_m$	Complex cosine of complex angle of refraction in substrate
D	**d**	Complex optical path length
R1S	r_{1s}	Fresnel reflection coefficient at film-air (or incident medium)interface. (For polarization normal to plane of incidence)
R1P	r_{1p}	Fresnel reflection coefficient at film-air (or incident medium) interface. (For polarization parallel to plane of incidence)
R2S	r_{2s}	Fresnel reflection coefficient at metal-film interfaee (normal polarization)
R2P	r_{2p}	Fresnel reflection coefficient at metal-film interface (parallel polarization)
RS	r_s	Overall reflection coefficient for polarization normal to plane of incidence
RP	r_p	Overall reflection coefficient for polarization parallel to plane of incidence
RHO	$\rho=r_p/r_s=\tan\psi\ e^{i\Delta}$	
TN3	$n_m - ik_m$	Complex refractive index of substrate
TN2	$n_f - ik_f$	Complex refractive index of film

Input Format for Program FILM

Card	Columns 1-10	11-20	21-30	31-40	41-50	51-70
1, 2	Title and comments (up to 80 columns each)					
3	n_o	λ_o	n_m	k_m		
4	n_{fi} (initial)	δn_f (increment)	n_{fm} (final)	k_{fi} (initial)	δk_f (increment)	k_{fm} (final)
5	L_i (initial)	δL (increment)	L_m (final)			
6	ϕ	P_m	A_m	ε_P	ε_A	Q

These six cards constitute a set. Any number of sets may follow. Three blank cards must follow the last set of data. Cards 1 and 2 of each set may contain any comments (or none at all) as desired. Their contents appear printed verbatim at the head of the output.

This program can be used to calculate theoretical values of P_c and A_c with changes in film thickness or with different film constants, by punching numbers greater than (or equal to) 90 for ε_A and a number greater than (or equal to) 180 for ε_P. Then the entries for P_m and A_m should be blank.

The program, together with a sample of output, is reproduced below.

FILM

```
           PROGRAM FILM (INPUT,OUTPUT)
      C    THIS PROGRAM USES AZIMUTH READINGS
      C    THIS PROGRAM CALCULATES THE THICKNESS AND COMPLEX REFRACTIVE
      C    INDEX OF A SINGLE ABSORBING FILM ON AN ABSORBING SUBSTRATE
      C    USING ELLIPSOMETER READINGS OF ZONE A3
           COMPLEX TN2, TN3, CPHI2, CPHI3, R1S, R1P, R2S, R2P, D, RS, RP
           DIMENSION TITLE (8), RANGE (8)                         ,RHO
         1 READ 2, TITLE,RANGE
         2 FORMAT (8A10/8A10)
 12      3 PRINT 4, TITLE,RANGE
         4 FORMAT (1H1, 8A10//8A10)
 22      5 READ 9, TN1,WL,TNS,TNKS
 36        IF (TN1) 3000, 3000, 6
 40      6 READ 10, TNI,DTN,TNM,TNKI,DTNK,TNKM
 60      7 READ 11, TI,DT,TM
 72      8 READ 12,PHI1,PM,AM,EPM,EAM,Q
         9 FORMAT (4F10.0)
        10 FORMAT (6F10.0)
        11 FORMAT (3F10.0)
        12 FORMAT (6F10.0)
        13 FORMAT (1H0,/6HPHI = ,F5.2,10X,4HN = ,F7.4, 10X, 13HWAVELENGTH
          C F5.0, 11H  ANGSTROMS//33H REFRACTIVE INDEX OF SUBSTRATE = , F
          C 2X, 4H-  I, F7.4)
        14 FORMAT (1H0, 27HREFRACTIVE INDEX OF FILM = , F7.4, 2X,
          C 4H-  I, F7.4//18H FILM THICKNESS = , F7.2, 10H ANGSTROMS,
          C //8H PSIC = , F10.5, 10X, 7HDELC = , F10.5,
          C //8H PSIM = , F10.5, 10X, 7HDELM = , F10.5)
       141 FORMAT (1H0, 5HPC = ,F10.5,10X,5HAC = ,F10.5,10X,4HQ = ,F5.2)
        15 FORMAT (1H0,  5HPM = ,F10.5,10X,, 5HAM = ,F10.5//33H NO SOLUT
          CWITHIN GIVEN LIMITS)
       151 FORMAT (1H0, 5HPM = ,F10.5,10X,5HAM = ,F10.5,10X,4HQ = ,F6.2)
112        IF (PM) 16,16,17
114     16 DELM=0.
115        PSIM=0.
116        GO TO 18
116     17 DELM=270.-2.*PM
121        PSIM=AM
123     18 EDELM=2.0*EPM
125        EPSIM=EAM
126        M = 1
127        PHI = 0.01745329252*PHI1
132        CP = COS(PHI)
133        SP = SIN(PHI)
135        TN3 = CMPLX(TNS,-TNKS)
141        CPHI3 = CSQRT(1.0 - TN1**2*SP**2/(TN3**2))
163        TN = TNI
165     20 TNK = TNKI
167     30 T = TI
171    100 TN2 = CMPLX(TN,-TNK)
174        CPHI2 = CSQRT(1.0 - TN1**2*SP**2/(TN2**2))
217        R1S = (TN1*CP - TN2*CPHI2)/(TN1*CP + TN2*CPHI2)
251        R1P =-(TN1*CPHI2 - TN2*CP)/(TN1*CPHI2 + TN2*CP)
302        R2S = (TN2*CPHI2 - TN3*CPHI3)/(TN2*CPHI2 + TN3*CPHI3)
341        R2P =-(TN2*CPHI3 - TN3*CPHI2)/(TN2*CPHI3 + TN3*CPHI2)
377        D = (0.0,1.0)*(4.0*3.1415927*T/WL)*TN2*CPHI2
415        RS= (R1S + R2S*CEXP(-D))/(1.0 + R1S*R2S*CEXP(-D))
454        RP = (R1P + R2P*CEXP(-D))/(1.0 + R1P*R2P*CEXP(-D))
```

```
513          RHO = RP/RS
523          PSIC = ATAN(CABS(RHO))/0.01745329252
527          DELC = ATAN2(AIMAG(RHO), REAL(RHO))/0.01745329252
536          IF (DELC) 140,140,150
540      140 DELC = DELC + 360.00
542      150 IF (EPSIM - ABS(PSIC - PSIM)) 400, 200, 200
547      200 IF (EDELM - ABS(DELC - DELM)) 400, 300, 300
554      300 PRINT 13, PHI1,TN1,WL,TNS,TNKS
572          PRINT 14, TN,TNK,T,PSIC,DELC,PSIM,DELM
614          PRINT 151,PM,AM,O
626          PC=(270.0-DELC)/2.0
631          AC=     PSIC
632          PRINT 141,PC,AC,O
644          M = 2
645      400 IF(TM -T) 600,600,500
650      500 T = T + DT
652          GO TO 100
653      600 IF(TNKM - TNK) 800,800,700
656      700 TNK = TNK + DTNK
660          GO TO 30
661      800 IF(TNM - TN) 1000,1000,900
664      900 TN = TN + DTN
666          GO TO 20
667     1000 GO TO (2000, 1) M
675     2000 PRINT 13, PHI1,TN1,WL,TNS,TNKS
713          PRINT 15,PM,AM
723          GO TO 1
724     3000 CONTINUE
725          END
```

Sample output, program FILM

```
 MGF2 ON CR          *** FILM  ***
ZONE A3 (AZIMUTH)

PHI = 75.00            N =  1.0000          WAVELENGTH =  5461  ANGSTROMS
 REFRACTIVE INDEX OF SUBSTRATE =   .9300  -  I 2.3900
 REFRACTIVE INDEX OF FILM =  1.3800  -  I-0.0000
 FILM THICKNESS =  400.00 ANGSTROMS
 PSIC =   41.11701          DELC =    55.78266
 PSIM =   41.11000          DELM =    55.80000
 PM =  107.10000          AM =    41.11000         Q =  45.00
 PC =  107.10867          AC =    41.11701         Q = 45.00
```

VI. FORTRAN IV Computer Program "A3PLOT"

This program calculates theoretical quantities of polarizer and analyzer values of the ellipsometer with changes in film thickness.* Depending on the code number M (see below), results are given as curves or tables.

The equation and variables used in this program are similar to those used in program "FILM".

As program "FILM" this program is only valid for zone A-3 (see Table I):

range of polarizer transmission azimuth	90-135°
range of analyzer transmission azimuth	0-90°
compensator circle realing	45°

*This program makes use of program "FPLOT" (see Chapter IX).

Input Format for Program A3PLOT

	Columns					
Card	1-9	10-19	20-29	30-39	40-49	50-59
1, 2 }	Title and comments (up to 80 columns)					
3	n_o	λ_o	n_m	k_m		
4	n_{fi} (initial)	δn_f (increment)	n_{fm} (final)	k_{fi} (initial)	δk_f (increment)	k_{fm} (final)
5	L_i	δL	L_m (limited to 200 points)			
6	ϕ	M				

These six cards constitute a set. Any number of sets may follow. In each set, the values of the optical constants of the film may be varied. Three blank cards must follow the last set of cards.

M is the code number. The integer used for M determines how the results will be presented.

M	Format of Results
0	Results will be tabulated and given as three curves a) ψ vs Δ curve with thickness as parameter b) A_c vs film thickness c) P_c vs film thickness
1	Results will be tabulated and only the ψ vs Δ curve is plotted
2	Results will be tabulated and two curves will be plotted a) A_c vs film thickness b) P_c vs film thickness
3	Results will be given only as three curves a) ψ vs Δ b) A_c vs film thickness c) P_c vs film thickness
4	Output has only the ψ vs Δ curve
5	Two curves will be given a) A_c vs film thickness b) P_c vs film thickness

The maximum number of data points for L (thickness) is 200. If the ψ vs thickness and Δ vs thickness curves are to be plotted, the maximum number is reduced to 101. The program "FILM" should be used instead, if only tabulated results are wanted.

This program "A3PLOT" has to utilize the subroutines "PRNPLT" and "PLSCAL" written by M. S. Itzkowitz to do the plotting of the curves. These two subroutines are library subroutines and they are stored in the computer (control data 7600 system) at Lawrence Berkeley Laboratory.

If the data are plotted, the scale of the thickness (x-axes) is divided into 100 parts from 0-10,000 A (increment (100 A), whereas the y-axes (P or A scale) is divided in 50 parts from 0-360° for P (increment 7.2°) and 0-180° (increment 3.6°) for A. The scales can be changed by using different "CALL PRNPLT"-cards. Cards numbers 670, 672, 774, 1052, 1464 of the program have the following form:

CALL PRNPLT(XPLOT, YPLOT, XMAX, XINCR, YMAX, YINCR, ISX, ISY, NPOINT)

with

XMAX	determines the upper limit of the x-axes (thickness)
XINCR	determines the increment of the x-values (increments of thickness)
YMAX	determines the upper limit of the y-axes (A, P-values)
YINCR	determines the increment of the y-values (increments of P, A-values).
ISX=0	means scaling of x-axes is done by programmer
ISX=1	means scaling of x-axes is done by computer
ISY=0	means scaling of y-axes is done by programmer
ISY=1	means scaling of y-axes is done by computer

In any case, the x-axes is divided into 100 parts; the y-axes into 50 parts.

A reproduction of the main program and the two subroutines is given below.

A3PLOT

```
               PROGRAM A3PLOT (INPUT,OUTPUT)
        C      THIS PROGRAM USES AZIMUTH READINGS
        C      THIS PROGRAM CALCULATES AC   AND PC   FROM FILM THICKNESS
        C      IT ALSO PLOTS AC   VERSUS PC   CURVE WITH FILM THICKNESS AS PA
        C      AND AC   VERSUS FILM THICKNESS, PC   VERSUS FILM THICKNESS.
        C      ZONE A3
               COMPLEX TN2, TN3, CPHI2, CPHI3, R1S, R1P, R2S, R2P, D, RS, RP, RHO
               DIMENSION TITLE (8), RANGE (8)
               DIMENSION XPLOT(200), YPLOT(200), ZPLOT(200)
             1 READ 2, TITLE,RANGE
             2 FORMAT (8A10/8A10)
   12        3 PRINT 4, TITLE,RANGE
             4 FORMAT (1H1, 8A10//8A10)
   22        5 READ 9, TN1,WL,TNS,TNKS
   36          IF (TN1) 3000, 3000, 6
   40        6 READ 10, TNI,DTN,TNM,TNKI,DTNK,TNKM
   60        7 READ 11, TI,DT,TM
   72          IF (TI.NE.0.0) TD=TM-TI
   75        8 READ 12, PHI1,M
             9 FORMAT (F9.0, 3F10.0)
            10 FORMAT (F9.0, 5F10.0)
            11 FORMAT (F9.0, 2F10.0)
            12 FORMAT (F9.0, I1 )
            13 FORMAT (1H0,/6HPHI = ,F5.2,10X,4HN = ,F7.4, 10X, 13HWAVELENGTH
              C F5.0, 11H  ANGSTROMS//33H REFRACTIVE INDEX OF SUBSTRATE = , F7.4,
              C 2X, 4H-  I, F7.4)
            14 FORMAT (1H0, 27HREFRACTIVE INDEX OF FILM = , F7.4, 2X,
              C 4H-  I, F7.4//18H FILM THICKNESS = , F8.2, 10H ANGSTROMS,
              C //8H   AC = , F10.5, 10X, 7H  PC = , F10.5)
            15 FORMAT (1H1)
            16 FORMAT (22HPSIC VERSUS DELC CURVE)
            17 FORMAT (6HPHI = ,F5.2,10X,4HN = ,F7.4,10X,13HWAVELENGTH = ,
              C F5.0,4H  A ,5X,13HNM  -  IKM = ,F7.4,2X,4H-  I,F7.4)
            18 FORMAT (13HNF  -  IKF = ,F7.4,2X,4H-  I,F7.4)
            19 FORMAT (26H PC  VERSUS FILM THICKNESS)
            21 FORMAT (26H AC  VERSUS FILM THICKNESS)
  105          PHI = 0.01745329252*PHI1
  107          CP = COS(PHI)
  111          SP = SIN(PHI)
  113          TN3 = CMPLX(TNS,-TNKS)
  117          CPHI3 = CSQRT(1.0 - TN1**2*SP**2/(TN3**2))
  141          TN = TNI
  143       20 TNK = TNKI
  145       30 T = TI
  146          NPOINT = 1
  150      100 TN2 = CMPLX(TN,-TNK)
  153          CPHI2 = CSQRT(1.0 - TN1**2*SP**2/(TN2**2))
  176          R1S = (TN1*CP - TN2*CPHI2)/(TN1*CP + TN2*CPHI2)
  230          R1P =-(TN1*CPHI2 - TN2*CP)/(TN1*CPHI2 + TN2*CP)
  261          R2S = (TN2*CPHI2 - TN3*CPHI3)/(TN2*CPHI2 + TN3*CPHI3)
  320          R2P =-(TN2*CPHI3 - TN3*CPHI2)/(TN2*CPHI3 + TN3*CPHI2)
  356          D = (0.0,1.0)*(4.0*3.1415927*T/WL)*TN2*CPHI2
  374          RS= (R1S + R2S*CEXP(-D))/(1.0 + R1S*R2S*CEXP(-D))
  433          RP = (R1P + R2P*CEXP(-D))/(1.0 + R1P*R2P*CEXP(-D))
  472          RHO = RP/RS
  502          PSIC = ATAN(CABS(RHO))/0.01745329252
  506          DELC = ATAN2(AIMAG(RHO), REAL(RHO))/0.01745329252
```

```
      IF (DELC) 140,140,150
  140 DELC = DELC + 360.00
  150 PC=(270.-DELC)/2.
      AC=PSIC
      IF(M.GT.2) GO TO 300
      PRINT 13, PHI1,TN1,WL,TNS,TNKS
      PRINT 14, TN,TNK,T,AC,PC
  300 XPLOT(NPOINT) = PC
      YPLOT(NPOINT) = AC
      IF(M.EQ.1.OR.M.EQ.4) GO TO 400
      IF(TI.EQ.0.0) GO TO 3500
      ZPLOT(NPOINT) = T - TD
      GO TO 400
 3500 ZPLOT(NPOINT) = T
  400 NPOINT = NPOINT + 1
      IF(TM -T) 600,600,500
  500 T = T + DT
      GO TO 100
  600 NPOINT = NPOINT - 1
      IF(M.EQ.2.OR.M.EQ.5) GO TO 1500
      PRINT 15
      PRINT 16
      PRINT 17, PHI1,TN1,WL,TNS,TNKS
      PRINT 18, TN,TNK
      XPLOT(NPOINT) = DELC
      YPLOT(NPOINT) = PSIC
      CALL PRNPLT(XPLOT,YPLOT,360.,5.0,90.,2.0,0.,0.,NPOINT)
      XPLOT(NPOINT) = PC
      YPLOT(NPOINT) = AC
      IF(M.EQ.1.OR.M.EQ.4) GO TO 1100
 1500 PRINT 15
      PRINT 21
      PRINT 17, PHI1,TN1,WL,TNS,TNKS
      PRINT 18, TN,TNK
      IF(TI.EQ.0.0) GO TO 3100
      PRINT 3300, TD
 3300 FORMAT (5HADD    ,F8.2,17HTO SCALE READINGS)
      CALL PRNPLT(ZPLOT,YPLOT,TM,10.,100.,2.0 ,0,0,NPOINT)
      GO TO 3400
 3100 CALL PRNPLT(ZPLOT,YPLOT,TM,10.,100.,2.0 ,0,0,NPOINT)
 3400 PRINT 15
      PRINT 19
      PRINT 17, PHI1,TN1,WL,TNS,TNKS
      PRINT 18, TN,TNK
      IF(TI.EQ.0.0) GO TO 3200
      PRINT 3300, TD
      CALL PRNPLT(ZPLOT,XPLOT,TM,10.,135.,1.0,0,0,NPOINT)
      GO TO 1100
 3200 CALL PRNPLT(ZPLOT,XPLOT,TM,10.,135.,1.0,0,0,NPOINT)
 1100 IF(TNKM - TNK) 800,800,700
  700 TNK = TNK + DTNK
      GO TO 30
  800 IF(TNM - TN) 1000,1000,900
  900 TN = TN + DTN
      GO TO 20
 1000 GO TO 1
 3000 CONTINUE
      END
```

PRNPLT

```
              SUBROUTINE PRNPLT(X,Y,XMAX,XINCR,YMAX,YINCR,ISX,ISY,NPTS)
        C  PRINTER PLOT ROUTINE        M.S.ITZKOWITZ     MAY,1967
        C
        C    PLOTS THE *NPTS* POINTS GIVEN BY *X(I),Y(I)* ON A 51 X 101 GRID
        C    USING A TOTAL OF 56 LINES ON THE PRINTER
        C      IF *ISX* OR *ISY* ARE NON-ZERO, THE CORRESPONDING MAXIMUM AND
        C        INCREMENTAL STEP SIZE ARE COMPUTED
        C      IF EITHER INCREMENTAL STEP SIZE IS ZERO, THE PROGRAM EXITS
        C      NEITHER OF THE INPUT ARRAYS ARE DESTROYED.  IF SCALING IS DONE
        C      THE CORRESPONDING NEW VALUES OF MAXIMUM AND STEP SIZE ARE RETU
        C
              DIMENSION X(NPTS),Y(NPTS),IGRID(105),XAXIS(11)
        C
              INTEGER BLANK,DOT,STAR,IGRID,PLUS
              DATA BLANK,DOT,STAR,PLUS / 1H ,1H.,1H*,1H+ /
        C
        901   FORMAT(14X,105A1)
        902   FORMAT(1XF10.3,2X,1H+,105A1,1H+)
        903   FORMAT(15X,103(1H.))
        904   FORMAT(7X,11(F10.0),2H (,I4,5H PTS)   )
        905   FORMAT(16X,11(1H+,9X))
        9800  FORMAT(46H1SCALING ERROR IN PRNPLT, EXECUTION TERMINATED )
        C
              IF(ISX.NE.0) CALL PLSCAL(X,XMAX,XINCR,NPTS,100)
   17         IF(ISY.NE.0) CALL PLSCAL(Y,YMAX,YINCR,NPTS,50)
   30         IF(XINCR.EQ.0..OR.YINCR.EQ.0.) GO TO 800
   42         YAXMIN=0.01*YINCR
   43         XAXMIN=0.01*XINCR
   44         IZERO=YMAX/YINCR+1.5
   47         JZERO=103.5-XMAX/XINCR
   51         IF(JZERO.GT.103.OR.JZERO.LT.4) JZERO=2
   63         PRINT 905
   67         PRINT 903
   76         DO 10 I=1,51
  103         IF ( I.NE.IZERO) GO TO 16
  104         DO 14 J=1,105
  112   14    IGRID(J)=PLUS
  113         GO TO 15
  117   16    DO 11 J=1,105
  125   11    IGRID(J)=BLANK
  132   15    IGRID(JZERO)=PLUS
  133         IGRID(104)=DOT
  136         IGRID(2)=DOT
  137         DO 12 K=1,NPTS
  140         ITEST =(YMAX-Y(K))/YINCR+1.5
  144         IF(ITEST .NE.I) GO TO 12
  146         J=103.5-(XMAX-X(K))/XINCR
  152         IF(J.GT.103)J=105
  156         IF(J.LT.3) J=1
  162         IGRID(J)=STAR
  164   12    CONTINUE
  167         IF(MOD(I,10).EQ.1) GO TO 13
  174         PRINT 901,IGRID
  201         GO TO 10
  205   13    YAXIS=YMAX-(I-1)*YINCR
  211         IF(ABS(YAXIS).LT.YAXMIN) YAXIS=0.
  216         PRINT 902,YAXIS,(IGRID(J),J=1,105)
```

```
232   10     CONTINUE
234          PRINT 903
240          PRINT 905
247          DO 20 M=1,11
254          XAXIS(M)=XMAX-XINCR*(FLOAT(11-M))*10.0
257          IF(ABS(XAXIS(M)).LT.XAXMIN)XAXIS(M)=0.
266   20     CONTINUE
270          PRINT 904,XAXIS,NPTS
300          RETURN
301   800    PRINT 9800
305          CALL EXIT
306          END
```

PLSCAL

```
              SUBROUTINE PLSCAL(V,VMAX,VINCR,NPTS,NDIVIS)
         C
         C     SCALING PROGRAM FOR USE WITH PRNPLT   M.S.ITZKOWITZ  MAY,1967
         C   THIS VERSION ADJUSTS THE FULL SCALE TO 2.5,5.0, OR 10. TIMES 10**N
         C   AND ADJUSTS THE MAXIMUM POINT TO AN INTEGER MULTIPLE OF 5*VINCR
         C
              DIMENSION V(NPTS)
         C
              VMIN=V(1)
  10          VMAX=V(1)
  11          DO 10 I=1,NPTS
  12          IF(V(I).LT.VMIN) VMIN=V(I)
  16          IF(V(I).GT.VMAX) VMAX=V(I)
  23          QRANGE=VMAX-VMIN
  25     10   CONTINUE
  27          IF(QRANGE.EQ.0.) GO TO 8000
  30          QRANGE=0.4342944*ALOG(QRANGE)
  32          IF(QRANGE)20,20,30
  37     30   IRANGE=QRANGE
  41          GO TO 40
  42     20   IRANGE=-QRANGE
  43          IRANGE=-IRANGE-1
  46     40   QRANGE=QRANGE-FLOAT(IRANGE)
  50          RANGE=10.**QRANGE
         C
         C   RANGE IS BETWEEN 1.0 AND 10.0
         C
  53     43   IF(RANGE.GT.2.5) GO TO 41
  57          RANGE=2.5
  57          GO TO 50
  60     41   IF(RANGE.GT.5.0) GO TO 42
  64          RANGE=5.0
  64          GO TO 50
  65     42   RANGE=10.0
  67     50   TRANGE=RANGE*(10.**IRANGE)
         C
         C    TRANGE IS NOW 2.5,5.0, OR 10.0 TIMES A POWER OF TEN
         C
  73          VINCR=TRANGE/FLOAT(NDIVIS)
  75          IF(VMAX)51,51,52
  77     52   IMAX=VMAX/(5.0*VINCR)
 101          XMAX=5.0*VINCR*FLOAT(IMAX+1)
 104          GO TO 53
 105     51   IMAX=-VMAX/(5.0*VINCR)
 110          XMAX=5.0*VINCR*FLOAT(-IMAX+1)
 113     53   IF(VMIN.GT.XMAX-TRANGE) GO TO 100
 120          RANGE=RANGE*2.0
 121          IF(RANGE-10.) 43,43,54
 124     54   RANGE=RANGE/10.
 126          IRANGE=IRANGE+1
 127          GO TO 43
 130    100   VMAX=XMAX
 131          VMIN=XMAX-TRANGE
 133          RETURN
 134   8000   PRINT 9800
       9800   FORMAT(45H1PLSCAL CALLED TO SCALE ARRAY WITH ZERO RANGE)
 143          CALL EXIT
 144          END
```

GOLD ON CHROMIUM *** A3PLOT ***

PC AND AC (OPT.5) VERSUS FILM THICKNESS (0 - 1000 A)

PHI = 75.00 N = 1.0000 WAVELENGTH = 5461 ANGSTROMS
REFRACTIVE INDEX OF SUBSTRATE = 2.9900 - I 2.3000
REFRACTIVE INDEX OF FILM = .3500 - I 2.3500
FILM THICKNESS = -0.00 ANGSTROMS
AC = 19.73136 PC = 88.28943

PHI = 75.00 N = 1.0000 WAVELENGTH = 5461 ANGSTROMS
REFRACTIVE INDEX OF SUBSTRATE = 2.9900 - I 2.3000
REFRACTIVE INDEX OF FILM = .3500 - I 2.3500
FILM THICKNESS = 50.00 ANGSTROMS
AC = 26.29669 PC = 90.91716

PHI = 75.00 N = 1.0000 WAVELENGTH = 5461 ANGSTROMS
REFRACTIVE INDEX OF SUBSTRATE = 2.9900 - I 2.3000
REFRACTIVE INDEX OF FILM = .3500 - I 2.3500
FILM THICKNESS = 100.00 ANGSTROMS
AC = 30.96695 PC = 92.84166

PHI = 75.00 N = 1.0000 WAVELENGTH = 5461 ANGSTROMS
REFRACTIVE INDEX OF SUBSTRATE = 2.9900 - I 2.3000
REFRACTIVE INDEX OF FILM = .3500 - I 2.3500
FILM THICKNESS = 150.00 ANGSTROMS
AC = 34.20930 PC = 94.34942

PHI = 75.00 N = 1.0000 WAVELENGTH = 5461 ANGSTROMS
REFRACTIVE INDEX OF SUBSTRATE = 2.9900 - I 2.3000
REFRACTIVE INDEX OF FILM = .3500 - I 2.3500
FILM THICKNESS = 200.00 ANGSTROMS
AC = 36.44506 PC = 95.54335

PHI = 75.00 N = 1.0000 WAVELENGTH = 5461 ANGSTROMS

REFRACTIVE INDEX OF SUBSTRATE = 2.9900 - I 2.3000

REFRACTIVE INDEX OF FILM = .3500 - I 2.3500

FILM THICKNESS = 250.00 ANGSTROMS

AC = 37.98865 PC = 96.48510

PHI = 75.00 N = 1.0000 WAVELENGTH = 5461 ANGSTROMS

REFRACTIVE INDEX OF SUBSTRATE = 2.9900 - I 2.3000

REFRACTIVE INDEX OF FILM = .3500 - I 2.3500

FILM THICKNESS = 300.00 ANGSTROMS

AC = 39.05905 PC = 97.22308

PHI = 75.00 N = 1.0000 WAVELENGTH = 5461 ANGSTROMS

REFRACTIVE INDEX OF SUBSTRATE = 2.9900 - I 2.3000

REFRACTIVE INDEX OF FILM = .3500 - I 2.3500

FILM THICKNESS = 350.00 ANGSTROMS

AC = 39.80513 PC = 97.79789

PHI = 75.00 N = 1.0000 WAVELENGTH = 5461 ANGSTROMS

REFRACTIVE INDEX OF SUBSTRATE = 2.9900 - I 2.3000

REFRACTIVE INDEX OF FILM = .3500 - I 2.3500

FILM THICKNESS = 400.00 ANGSTROMS

AC = 40.32759 PC = 98.24346

PHI = 75.00 N = 1.0000 WAVELENGTH = 5461 ANGSTROMS

REFRACTIVE INDEX OF SUBSTRATE = 2.9900 - I 2.3000

REFRACTIVE INDEX OF FILM = .3500 - I 2.3500

FILM THICKNESS = 450.00 ANGSTROMS

AC = 40.69481 PC = 98.58760

PHI = 75.00 N = 1.0000 WAVELENGTH = 5461 ANGSTROMS

REFRACTIVE INDEX OF SUBSTRATE = 2.9900 - I 2.3000

REFRACTIVE INDEX OF FILM = .3500 - I 2.3500

FILM THICKNESS = 500.00 ANGSTROMS

AC = 40.95360 PC = 98.85264

PHI = 75.00 N = 1.0000 WAVELENGTH = 5461 ANGSTROMS
REFRACTIVE INDEX OF SUBSTRATE = 2.9900 - I 2.3000
REFRACTIVE INDEX OF FILM = .3500 - I 2.3500
FILM THICKNESS = 550.00 ANGSTROMS
AC = 41.13624 PC = 99.05631

PHI = 75.00 N = 1.0000 WAVELENGTH = 5461 ANGSTROMS
REFRACTIVE INDEX OF SUBSTRATE = 2.9900 - I 2.3000
REFRACTIVE INDEX OF FILM = .3500 - I 2.3500
FILM THICKNESS = 600.00 ANGSTROMS
AC = 41.26518 PC = 99.21254

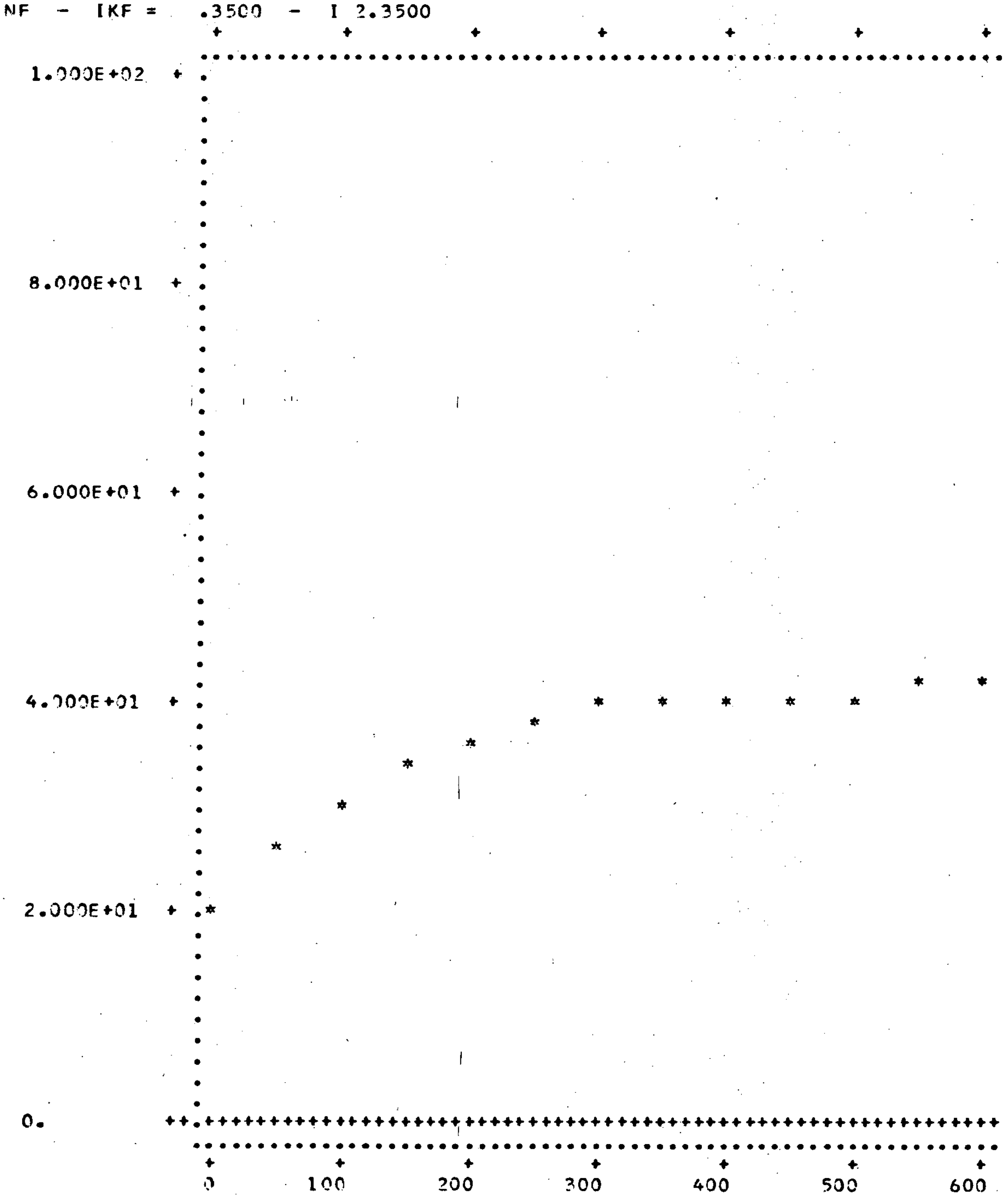
PHI = 75.00 N = 1.0000 WAVELENGTH = 5461 ANGSTROMS
REFRACTIVE INDEX OF SUBSTRATE = 2.9900 - I 2.3000
REFRACTIVE INDEX OF FILM = .3500 - I 2.3500
FILM THICKNESS = 650.00 ANGSTROMS
AC = 41.35616 PC = 99.33217

PHI = 75.00 N = 1.0000 WAVELENGTH = 5461 ANGSTROMS
REFRACTIVE INDEX OF SUBSTRATE = 2.9900 - I 2.3000
REFRACTIVE INDEX OF FILM = .3500 - I 2.3500
FILM THICKNESS = 700.00 ANGSTROMS
AC = 41.42025 PC = 99.42365

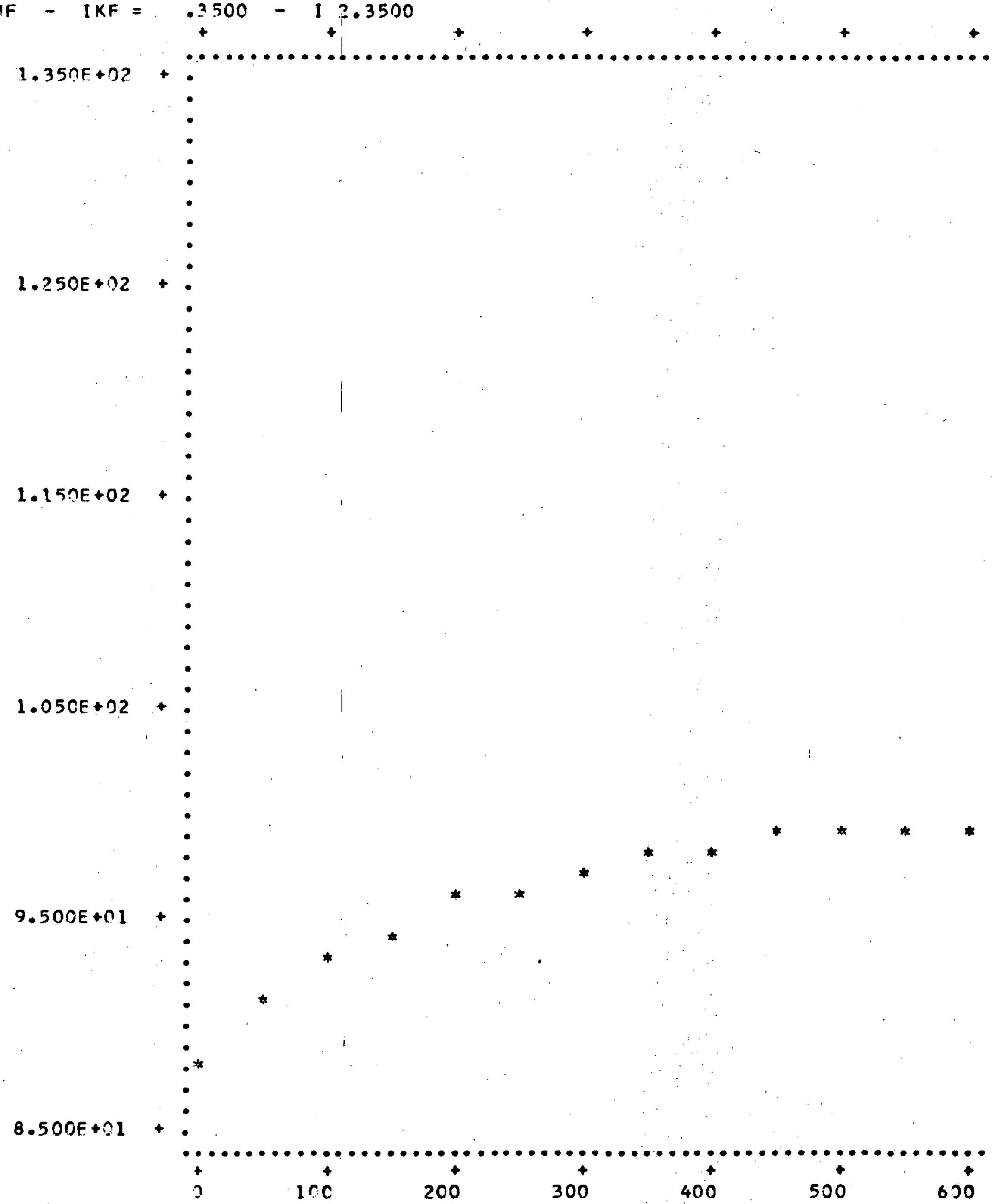
PHI = 75.00 N = 1.0000 WAVELENGTH = 5461 ANGSTROMS
REFRACTIVE INDEX OF SUBSTRATE = 2.9900 - I 2.3000
REFRACTIVE INDEX OF FILM = .3500 - I 2.3500
FILM THICKNESS = 750.00 ANGSTROMS
AC = 41.46528 PC = 99.49350

PHI = 75.00 N = 1.0000 WAVELENGTH = 5461 ANGSTROMS
REFRACTIVE INDEX OF SUBSTRATE = 2.9900 - I 2.3000
REFRACTIVE INDEX OF FILM = .3500 - I 2.3500

AC VERSUS FILM THICKNESS
PHI = 75.00 N = 1.0000 WAVELENGTH = 5461 A NM - IK
NF - IKF = .3500 - I 2.3500



PC VERSUS FILM THICKNESS
PHI = 75.00 N = 1.0000 WAVELENGTH = 5461 A NM - IK
NF - IKF = .3500 - I 2.3500



VII. FORTRAN IV Computer Program "PSIDEL"

This program has been written to convert ellipsometer azimuth-readings into relative phase Δ and amplitude parameter ψ. According to Table I , it determines the zone of measurement and provides two or four-zone averages.

Variables Used in the Program

Name	Symbol	Description
AM	A_m	Azimuth reading of analyzer
PM	P_m	Azimuth reading of polarizer
Q	Q	Azimuth reading of compensator
DELM	Δ	Relative phase change (deg)
PSIM	ψ	Arctangent of relative amplitude attenuation (deg)
N		Quantity of zones, over which one averages (4-zone measurement N = 4)

Input Format

Card	Columns 1-10	Columns 11-20	Columns 21-30
1	Title (up to 80 columns)		
2	N		
3	P_1	A_1	Q_1
4	P_2	A_2	Q_1
5	P_3	A_3	Q_2
6	P_4	A_4	Q_2

These 5 cards constitute 1 set for a 4-zone measurement. In case of a 2(1)-zone measurement, one set consists of only 4(3) cards. Two blank cards must follow the last set of data. The program, together with a sample output is reproduced below.

This program can be used as a subroutine in connection with program "CMOC", "OZOM" or "LAYER" in order to avoid the tedious use of the conversion table (Table I). Program "LAYER" was described by Gu,[1] but can also be found in the Appendix.

PSIDEL

```
              PROGRAM PSIDEL (INPUT,OUTPUT)
        C     THIS PROGRAM USES AZIMUTH READINGS
        C     THIS PROGRAM COMPUTES PSI AND DEL FROM ELLIPSOMETER READINGS A
        C     P FROM ONE,TWO OR FOUR ZONES                                   ND
              DIMENSION TITLE (8)
              EQUIVALENCE (PM,P),(AM,A)
         7000 CONTINUE
              READ 8,TITLE
            8 FORMAT (8A10)
   10         PRINT 9,TITLE
            9 FORMAT (1H1,8A10)
   16         P1=0.0
   17         P2=0.0
   17         P3=0.0
   20         P4=0.0
   20         A4=0.0
   21         A3=0.0
   21         A2=0.0
   22         A1=0.0
   23         READ 6,N
            6 FORMAT (I1)
   30         IF (N) 110,110,10
   32      10 DO 99 J=1,N
   34       1 READ 11,PM,AM,Q
           11 FORMAT (3F10.0)
   46       7 PRINT 207,PM,AM,Q
   60         PM=PM + 90.
   62         AM=AM + 90.
   64         Q=Q + 90.
   65         IF (P-180.0) 5,5,2
   70       2 P=P-180.0
   72       5 CONTINUE
   72         IF (A-180.0) 4,4,3
   75       3 A=A-180.0
   77       4 CONTINUE
   77         IF (Q-180.) 13,13,12
  102      12 Q=Q-180.
  104      13 CONTINUE
  104         IF (Q-45.0) 105,20,39
  107      20 IF (P-45.0) 21,21,22
  112      21 IF (A-90.0) 63,63,83
  115      22 IF (P-90.0) 23,23,24
  120      23 IF (A-90.0) 74,74,54
  123      24 IF (P-135.0) 25,25,26
  126      25 IF (A-90.0) 81,81,61
  131      26 IF (A-90.0) 52,52,72
  134      39 IF (Q-135.0) 40,40,105
  137      40 IF (P-45.0) 41,41,42
  142      41 IF (A-90.0) 73,73,53
  145      42 IF (P-90.0) 43,43,44
  150      43 IF (A-90.0) 64,64,84
  153      44 IF (P-135.0) 45,45,46
  156      45 IF (A-90.0) 51,51,71
  161      46 IF (A-90.0) 82,82,62
  164      51 P1=270.0-2.0*P
  167         A1=90.0-A
  171         GO TO 99
```

```
172      52 P2=2.0*P-270.0
175         A2=90.0-A
177         GO TO 99
200      53 P3=90.0-2.0*P
203         A3=A-90.0
205         GO TO 99
205      54 P4=2.0*P-90.0
210         A4=A-90.0
212         GO TO 99
212      61 P1=2.0*P-90.0
215         A1=A-90.0
217         GO TO 99
217      62 P2=450.0-2.0*P
222         A2=A-90.0
224         GO TO 99
225      63 P3=2.0*P+90.0
230         A3=90.0-A
232         GO TO 99
232      64 P4=270.0-2.0*P
235         A4=90.0-A
237         GO TO 99
240      71 P1=450.0-2.0*P
243         A1=A-90.0
245         GO TO 99
246      72 P2=2.0*P-90.0
251         A2=A-90.0
253         GO TO 99
253      73 P3=270.0-2.0*P
256         A3=90.0-A
260         GO TO 99
261      74 P4=2.0*P+90.0
264         A4=90.0-A
266         GO TO 99
266      81 P1=2.0*P+90.0
271         A1=90.0-A
273         GO TO 99
273      82 P2=630.0-2.0*P
276         A2=90.0-A
300         GO TO 99
301      83 P3=2.0*P+270.0
304         A3=A-90.0
306         GO TO 99
307      84 P4=450.0-2.0*P
312         A4=A-90.0
314         GO TO 99
315     105 PRINT 208,Q
        208 FORMAT (1H0,4HQ = ,F5.2 //11HNO SOLUTION)
323      99 CONTINUE
326     100 DELM=(P1+P2 +P3+P4)/4.0
333         PSIM=(A1+A2+A3+A4)/4.0
337         IF (N.EQ.1) GO TO 102
342         IF (N.EQ.2) GO TO 103
343         IF (N.EQ.4) GO TO 104
345     102 DELM=DELM*4.0
347         PSIM=PSIM*4.0
350         GO TO 104
350     103 DELM=DELM*2.0
352         PSIM=PSIM*2.0
```

```
353      104 PRINT 204,P1,P2,P3,P4
367          PRINT 205,A1,A2,A3,A4
403          PRINT 206,DELM,PSIM
         204 FORMAT (1H0,5HP1 = ,F10.5,10X,5HP2 = ,F10.5,10X,5HP3 = ,F10.5,
            25HP4 = ,F10.5)
         205 FORMAT (1H0,5HA1 = ,F10.5,10X,5HA2 = ,F10.5,10X,5HA3 = ,F10.5,
            25HA4 = ,F10.5//)
         206 FORMAT (1H0,7HDELM = ,F10.5,10X,7HPSIM = ,F10.5)
         207 FORMAT (1H0,5HPM = ,F10.5,10X,5HAM = ,F10.5,10X,4HQ = ,F6.2)
413          GO TO 7000
414      110 CONTINUE
415          END
```

MGF2 ON CR (3.48) *** PSIDEL ****

PM = 69.92700	AM = 140.71900	Q = 135.00	
PM = 159.71800	AM = 36.81200	Q = 135.00	
PM = 18.87500	AM = 142.47100	Q = 45.00	
PM = 108.70600	AM = 38.42400	Q = 45.00	
P1 = 52.25000	P2 = 49.85400	P3 = 52.58800	P4
A1 = 37.52900	A2 = 39.28100	A3 = 38.42400	A4

DELM = 51.03200 PSIM = 38.01150

VIII. FORTRAN IV Computer Program "LAYER"

The program "LAYER" finds the thickness and complex refractive index of a single, absorbing film on an absorbing substrate.* It does so by systematically combining all prescribed values of film thickness L and refractive index $n_f - ik_f$ and calculating the Δ and ψ for each combination. Whenever a particular combination of L, n_f and k_f yields agreement with the experimentally determined quantities Δ and ψ within a specified error ε_Δ and ε_ψ, this combination appears in the output as a solution.

Input Format for Program "LAYER"

Card	Col. 1	Col. 10	Col. 20	Col. 30	Col. 40	Col. 50
1, 2	Title and comments (up to 80 columns each)					
3	n_o	λ_o	n_m	k_m		
4	n_{fi} (initial)	δn_f (increment)	n_{fm} (final)	k_{fi} (initial)	δk_f (increment)	k_{fm} (final)
5	L_i (initial)	δL (increment)	L_m (final)			
6	ϕ	ψ	Δ	ε_ψ	ε_Δ	

These six cards constitute a set. Any number of sets may follow. Three blank cards must follow the last set of data. Cards 1 and 2 of each set may contain any comments (or none at all) as desired. Their contents appear printed verbatim in the head of the output.

This program can be used to calculate theoretical values of Δ and ψ, with changes in film thickness or with different film constants, by punching numbers greater than (or equal to) 90 for ε_Δ and a number

*Based on an earlier FORTRAN II program "FILM".[14]

greater than (or equal to) 360 for ε_Δ. Entries for ψ and Δ can be blank or any values such as 0.0.

The program, together with a sample of output, is reproduced on the following pages.

LAYER

```
                 PROGRAM LAYER (INPUT,OUTPUT)
           C     THIS PROGRAM IS INDEPENDENT OF ANGLE READINGS
           C     THIS PROGRAM CALCULATES THE THICKNESS AND COMPLEX REFRACTIVE
           C     INDEX OF A SINGLE ABSORBING FILM ON AN ABSORBING SUBSTRATE
                 COMPLEX TN2, TN3, CPHI2, CPHI3, R1S, R1P, R2S, R2P, D, RS, RP, RHO
                 DIMENSION TITLE (8), RANGE (8)
               1 READ 2, TITLE,RANGE
               2 FORMAT (8A10/8A10)
     12        3 PRINT 4, TITLE,RANGE
               4 FORMAT (1H1, 8A10//8A10)
     22        5 READ 9, TN1,WL,TNS,TNKS
     36          IF (TN1) 3000, 3000, 6
     40        6 READ 10, TNI,DTN,TNM,TNKI,DTNK,TNKM
     60        7 READ 11, TI,DT,TM
     72        8 READ 12, PHI1,PSIM,DELM,EPSIM,EDELM
               9 FORMAT (F9.0, 3F10.0)
              10 FORMAT (F9.0, 5F10.0)
              11 FORMAT (F9.0, 2F10.0)
              12 FORMAT (F9.0, 4F10.0)
              13 FORMAT (1H0,/6HPHI = ,F5.2,10X,4HN = ,F7.4, 10X, 13HWAVELENGTH = ,
                C F5.0, 11H  ANGSTROMS//33H REFRACTIVE INDEX OF SUBSTRATE = , F7.4,
                C 2X, 4H-  I, F7.4)
              14 FORMAT (1H0, 27HREFRACTIVE INDEX OF FILM = , F7.4, 2X,
                C 4H-  I, F7.4//18H FILM THICKNESS = , F7.2, 10H ANGSTROMS,
                C //8H PSIC = , F10.5, 10X, 7HDELC = , F10.5,
                C //8H PSIM = , F10.5, 10X, 7HDELM = , F10.5)
              15 FORMAT (1H0, 7HPSIM = , F10.5,10X,  7HDELM = , F10.5//32H NO SOLUT
                CION WITHIN GIVEN LIMITS)
    110          M = 1
    111          PHI = 0.01745329252*PHI1
    113          CP = COS(PHI)
    115          SP = SIN(PHI)
    117          TN3 = CMPLX(TNS,-TNKS)
    123          CPHI3 = CSQRT(1.0 - TN1**2*SP**2/(TN3**2))
    145          TN = TNI
    147       20 TNK = TNKI
    151       30 T = TI
    153      100 TN2 = CMPLX(TN,-TNK)
    156          CPHI2 = CSQRT(1.0 - TN1**2*SP**2/(TN2**2))
    201          R1S = (TN1*CP - TN2*CPHI2)/(TN1*CP + TN2*CPHI2)
    233          R1P =-(TN1*CPHI2 - TN2*CP)/(TN1*CPHI2 + TN2*CP)
    264          R2S = (TN2*CPHI2 - TN3*CPHI3)/(TN2*CPHI2 + TN3*CPHI3)
    323          R2P =-(TN2*CPHI3 - TN3*CPHI2)/(TN2*CPHI3 + TN3*CPHI2)
    361          D = (0.0,1.0)*(4.0*3.1415927*T/WL)*TN2*CPHI2
    377          RS= (R1S + R2S*CEXP(-D))/(1.0 + R1S*R2S*CEXP(-D))
    436          RP = (R1P + R2P*CEXP(-D))/(1.0 + R1P*R2P*CEXP(-D))
    475          RHO = RP/RS
    505          PSIC = ATAN(CABS(RHO))/0.01745329252
    511          DELC = ATAN2(AIMAG(RHO), REAL(RHO))/0.01745329252
    520          IF (DELC) 140,140,150
    522      140 DELC = DELC + 360.00
    524      150 IF (EPSIM - ABS(PSIC - PSIM)) 400, 200, 200
    531      200 IF (EDELM - ABS(DELC - DELM)) 400, 300, 300
    536      300 PRINT 13, PHI1,TN1,WL,TNS,TNKS
    554          PRINT 14, TN,TNK,T,PSIC,DELC,PSIM,DELM
    576          M = 2
    577      400 IF(TM -T) 600,600,500
```

```
  500 T = T + DT
      GO TO 100
  600 IF(TNKM - TNK) 800,800,700
  700 TNK = TNK + DTNK
      GO TO 30
  800 IF(TNM - TN) 1000,1000,900
  900 TN = TN + DTN
      GO TO 20
 1000 GO TO (2000, 1) M
 2000 PRINT 13, PHI1,TN1,WL,TNS,TNKS
      PRINT 15, PSIM,DELM
      GO TO 1
 3000 CONTINUE
      END
```

Sample output, program LAYER

```
 CU2O ON CU          *** LAYER    ***
TABLE 0 - 90 A

PHI = 75.00              N =  1.0000             WAVELENGTH =  5461  ANGSTROMS
 REFRACTIVE INDEX OF SUBSTRATE =   .9300  -  I 2.3900
 REFRACTIVE INDEX OF FILM =  2.7500  -  I  .1950
 FILM THICKNESS =    0.00 ANGSTROMS
 PSIC =   36.00128           DELC =   72.80712
 PSIM =   -0.00000           DELM =   -0.00000

PHI = 75.00              N =  1.0000             WAVELENGTH =  5461  ANGSTROMS
 REFRACTIVE INDEX OF SUBSTRATE =   .9300  -  I 2.3900
 REFRACTIVE INDEX OF FILM =  2.7500  -  I  .1950
 FILM THICKNESS =   30.00 ANGSTROMS
 PSIC =   36.39501           DELC =   65.76699
 PSIM =   -0.00000           DELM =   -0.00000

PHI = 75.00              N =  1.0000             WAVELENGTH =  5461  ANGSTROMS
 REFRACTIVE INDEX OF SUBSTRATE =   .9300  -  I 2.3900
 REFRACTIVE INDEX OF FILM =  2.7500  -  I  .1950
 FILM THICKNESS =   60.00 ANGSTROMS
 PSIC =   36.88396           DELC =   59.31852
 PSIM =   -0.00000           DELM =   -0.00000
```

IX. FORTRAN IV Computer Program "FPLOT"[1]

The program "FPLOT" (Film Plot) calculates theoretical quantities of ψ and Δ with changes in film thickness. Depending on the code number M, results are tabulated (as program LAYER) or given as curves or both.

Input data for program "FPLOT" are arranged on cards as illustrated below:

Card	Col. 1	Col. 10	Col. 20	Col. 30	Col. 40	Col. 50
1, 2	Title and comments (up to 80 columns)					
3	n_o	λ_o	n_m	k_m		
4	n_{fi} (initial)	δn_f (increment)	n_{fm} (final)	k_{fi} (initial)	δk_f (increment)	k_{fm}
5	L_i	δL	L_m (limited to 200 points)			
6	ϕ	M				

These six cards constitute a set. Any number of sets may follow. In each set, the values of the optical constants of the film may be varied in increments if one desired. Three blank cards must follow the last set of cards.

M is the code number. The integer used for M determines how the results will be presented.

M	Format of Results
0	Results will be tabulated and given as three curves a) ψ vs Δ curve with thickness as parameter b) ψ vs film thickness c) Δ vs film thickness
1	Results will be tabulated only the ψ vs Δ curve is plotted
2	Results will be tabulated and two curves will be plotted a) ψ vs film thickness b) Δ vs film thickness
3	Results will be given only as three curves a) ψ vs Δ b) ψ vs film thickness c) Δ vs film thickness
4	Output has only the ψ vs Δ curve
5	Two curves will be given a) ψ vs film thickness b) Δ vs film thickness

The maximum number of data points for L (thickness) is 200. If the ψ vs thickness and Δ vs thickness curves are to be plotted, the maximum number is reduced to 101. The program "LAYER" should be used instead, if only tabulated results are wanted.

This program "FPLOT" has to utilize the subroutines "PRNPLT" and "PLSCAL" written by M. S. Itzkowitz to do the plotting of the curves. These two subroutines are library subroutines and they are stored in the computer (control data 7600 system).

A reproduction of the main program and the two subroutines is given on the following pages. A sample of the output curves is also given.

EPLOT

```
              PROGRAM EPLOT (INPUT,OUTPUT)
       C      THIS PROGRAM IS INDEPENDENT OF ANGLE READINGS
       C      THIS PROGRAM CALCULATES DELC AND PSIC FROM FILM THICKNESS
       C      IT ALSO PLOTS PSIC VERSUS DELC CURVE WITH FILM THICKNESS AS PARAMETER
       C      AND PSIC VERSUS FILM THICKNESS, DELC VERSUS FILM THICKNESS.
              COMPLEX TN2, TN3, CPHI2, CPHI3, R1S, R1P, R2S, R2P, D, RS, RP, RHO
              DIMENSION TITLE (8), RANGE (8)
              DIMENSION XPLOT(200), YPLOT(200), ZPLOT(200)
            1 READ 2, TITLE,RANGE
            2 FORMAT (8A10/8A10)
 12         3 PRINT 4, TITLE,RANGE
            4 FORMAT (1H1, 8A10//8A10)
 22         5 READ 9, TN1,WL,TNS,TNKS
 36           IF (TN1) 3000, 3000, 6
 40         6 READ 10, TNI,DTN,TNM,TNKI,DTNK,TNKM
 60         7 READ 11. TI,DT,TM
 72           IF (TI.NE.0.0) TD=TM-TI
 75         8 READ 12, PHI1,M
            9 FORMAT (F9.0, 3F10.0)
           10 FORMAT (F9.0, 5F10.0)
           11 FORMAT (F9.0, 2F10.0)
           12 FORMAT (F9.0, I1 )
           13 FORMAT (1H0,/6HPHI = ,F5.2,10X,4HN = ,F7.4, 10X, 13HWAVELENGTH = ,
             C F5.0, 11H  ANGSTROMS//33H REFRACTIVE INDEX OF SUBSTRATE = , F7.4,
             C 2X, 4H-  I, F7.4)
           14 FORMAT (1H0, 27HREFRACTIVE INDEX OF FILM = , F7.4, 2X,
             C 4H-  I, F7.4//18H FILM THICKNESS = , F8.2, 10H ANGSTROMS,
             C //8H PSIC = , F10.5, 10X, 7HDELC = , F10.5)
           15 FORMAT (1H1)
           16 FORMAT (22HPSIC VERSUS DELC CURVE)
           17 FORMAT (6HPHI = ,F5.2,10X,4HN = ,F7.4,10X,13HWAVELENGTH = ,
             C F5.0,4H  A ,5X,13HNM  -  IKM = ,F7.4,2X,4H-  I,F7.4)
           18 FORMAT (13HNF  -  IKF = ,F7.4,2X,4H-  I,F7.4)
           19 FORMAT (26HDELC VERSUS FILM THICKNESS)
           21 FORMAT (26HPSIC VERSUS FILM THICKNESS)
 105          PHI = 0.01745329252*PHI1
 107          CP = COS(PHI)
 111          SP = SIN(PHI)
 113          TN3 = CMPLX(TNS,-TNKS)
 117          CPHI3 = CSQRT(1.0 - TN1**2*SP**2/(TN3**2))
 141          TN = TNI
 143       20 TNK = TNKI
 145       30 T = TI
 146          NPOINT = 1
 150      100 TN2 = CMPLX(TN,-TNK)
 153          CPHI2 = CSQRT(1.0 - TN1**2*SP**2/(TN2**2))
 176          R1S = (TN1*CP - TN2*CPHI2)/(TN1*CP + TN2*CPHI2)
 230          R1P =-(TN1*CPHI2 - TN2*CP)/(TN1*CPHI2 + TN2*CP)
 261          R2S = (TN2*CPHI2 - TN3*CPHI3)/(TN2*CPHI2 + TN3*CPHI3)
 320          R2P =-(TN2*CPHI3 - TN3*CPHI2)/(TN2*CPHI3 + TN3*CPHI2)
 356          D = (0.0,1.0)*(4.0*3.1415927*T/WL)*TN2*CPHI2
 374          RS= (R1S + R2S*CEXP(-D))/(1.0 + R1S*R2S*CEXP(-D))
 433          RP = (R1P + R2P*CEXP(-D))/(1.0 + R1P*R2P*CEXP(-D))
 472          RHO = RP/RS
 502          PSIC = ATAN(CABS(RHO))/0.01745329252
 506          DELC = ATAN2(AIMAG(RHO), REAL(RHO))/0.01745329252
 515          IF (DELC) 140,140,150
```

```
 517     140 DELC = DELC + 360.00
 521     150 IF(M.GT.2) GO TO 300
 525         PRINT 13, PHI1,TN1,WL,TNS,TNKS
 542         PRINT 14, TN,TNK,T,PSIC,DELC
 561     300 XPLOT(NPOINT) = DELC
 562         YPLOT(NPOINT) = PSIC
 564         IF(M.EQ.1.OR.M.EQ.4) GO TO 400
 574         IF(TI.EQ.0.0) GO TO 3500
 575         ZPLOT(NPOINT) = T - TD
 600         GO TO 400
 600    3500 ZPLOT(NPOINT) = T
 602     400 NPOINT = NPOINT + 1
 604         IF(TM -T) 600,600,500
 607     500 T = T + DT
 611         GO TO 100
 612     600 NPOINT = NPOINT - 1
 614         IF(M.EQ.2.OR.M.EQ.5) GO TO 1500
 623         PRINT 15
 626         PRINT 16
 632         PRINT 17, PHI1,TN1,WL,TNS,TNKS
 650         PRINT 18, TN,TNK
 660         CALL PRNPLT(XPLOT,YPLOT,360.,5.0,90.,2.0,0.,0.,NPOINT)
 671         IF(M.EQ.1.OR.M.EQ.4) GO TO 1100
 701    1500 PRINT 15
 705         PRINT 21
 711         PRINT 17, PHI1,TN1,WL,TNS,TNKS
 727         PRINT 18, TN,TNK
 737         IF(TI.EQ.0.0) GO TO 3100
 740         PRINT 3300, TD
        3300 FORMAT (5HADD  ,F8.2,17HTO SCALE READINGS)
 746         CALL PRNPLT(ZPLOT,YPLOT,TD,100.,90.,2.,0.,0.,NPOINT)
 757         GO TO 3400
 760    3100 CALL PRNPLT(ZPLOT,YPLOT,TM,100.,90.,2.,0.,0.,NPOINT)
 771    3400 PRINT 15
 775         PRINT 19
1001         PRINT 17, PHI1,TN1,WL,TNS,TNKS
1017         PRINT 18, TN,TNK
1027         IF(TI.EQ.0.0) GO TO 3200
1030         PRINT 3300, TD
1036         CALL PRNPLT(ZPLOT,XPLOT,TD,100.,360.,10.,0.,0.,NPOINT)
1047         GO TO 1100
1050    3200 CALL PRNPLT(ZPLOT,XPLOT,TM,100.,360.,10.,0.,0.,NPOINT)
1061    1100 IF(TNKM - TNK) 800,800,700
1064     700 TNK = TNK + DTNK
1066         GO TO 30
1067     800 IF(TNM - TN) 1000,1000,900
1072     900 TN = TN + DTN
1074         GO TO 20
1075    1000 GO TO 1
1076    3000 CONTINUE
1077         END
```

PROGRAM LENGTH INCLUDING I/O BUFFERS

03667

PRNPLT

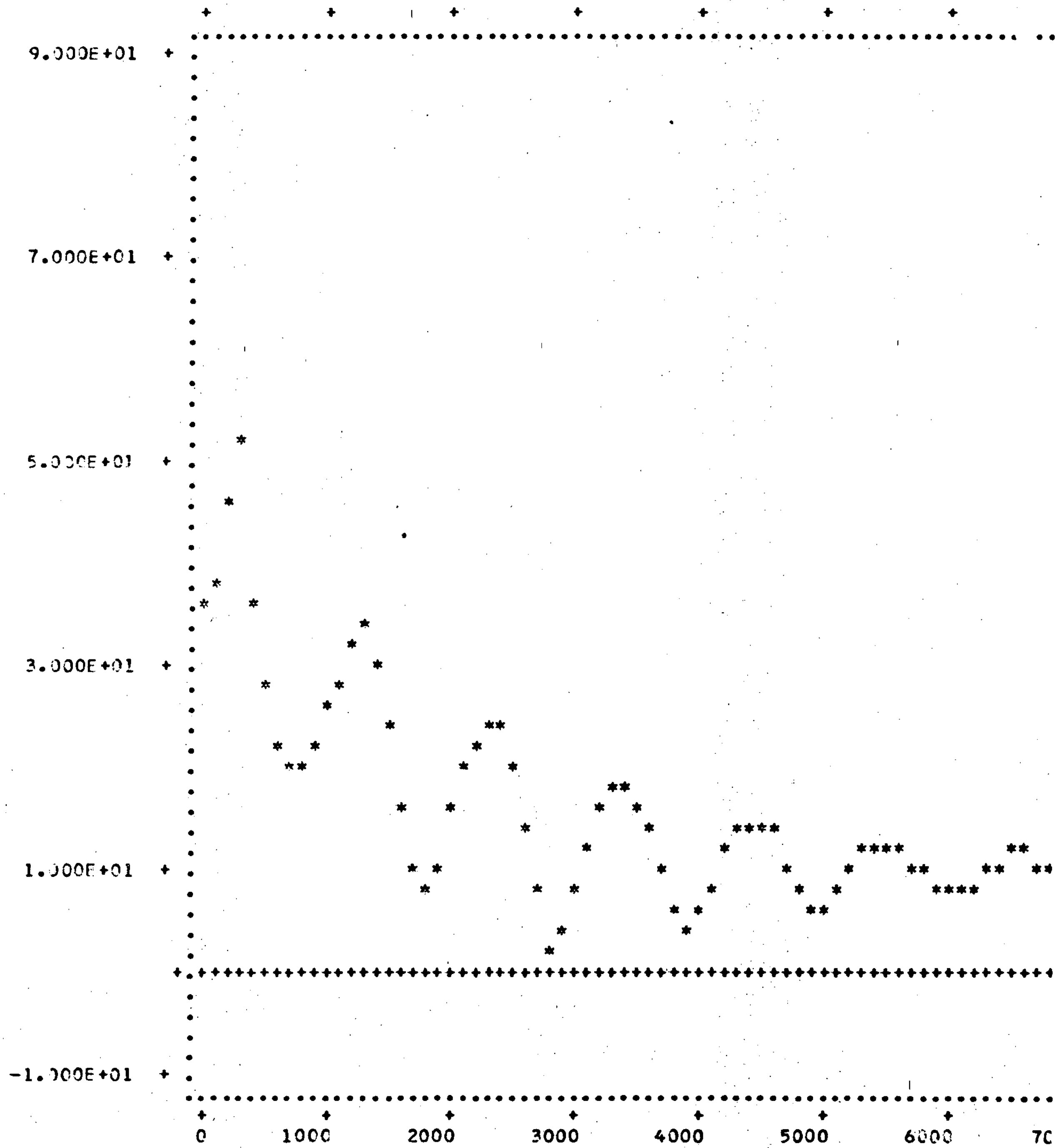
```
              SUBROUTINE PRNPLT(X,Y,XMAX,XINCR,YMAX,YINCR,ISX,ISY,NPTS)
        C   PRINTER PLOT ROUTINE           M.S.ITZKOWITZ      MAY,1967
        C
        C    PLOTS THE *NPTS* POINTS GIVEN BY *X(I),Y(I)* ON A 51 X 101 GRID
        C    USING A TOTAL OF 56 LINES ON THE PRINTER
        C       IF *ISX* OR *ISY* ARE NON-ZERO, THE CORRESPONDING MAXIMUM AND
        C        INCREMENTAL STEP SIZE ARE COMPUTED
        C       IF EITHER INCREMENTAL STEP SIZE IS ZERO, THE PROGRAM EXITS
        C       NEITHER OF THE INPUT ARRAYS ARE DESTROYED.  IF SCALING IS DONE
        C       THE CORRESPONDING NEW VALUES OF MAXIMUM AND STEP SIZE ARE RETURNED
        C
              DIMENSION X(NPTS),Y(NPTS),IGRID(105),XAXIS(11)
        C
              INTEGER BLANK,DOT,STAR,IGRID,PLUS
              DATA BLANK,DOT,STAR,PLUS / 1H ,1H.,1H*,1H+ /
        C
        901   FORMAT(14X,105A1)
        902   FORMAT(1XF10.3,2X,1H+,105A1,1H+)
        903   FORMAT(15X,103(1H.))
        904   FORMAT(7X,11(F10.0),2H (,I4,5H PTS)  )
        905   FORMAT(16X,11(1H+,9X))
        9800  FORMAT(46H1SCALING ERROR IN PRNPLT, EXECUTION TERMINATED )
        C
              IF(ISX.NE.0) CALL PLSCAL(X,XMAX,XINCR,NPTS,100)
   17         IF(ISY.NE.0) CALL PLSCAL(Y,YMAX,YINCR,NPTS,50)
   30         IF(XINCR.EQ.0..OR.YINCR.EQ.0.) GO TO 800
   42         YAXMIN=0.01*YINCR
   43         XAXMIN=0.01*XINCR
   44         IZERO=YMAX/YINCR+1.5
   47         JZERO=103.5-XMAX/XINCR
   51         IF(JZERO.GT.103.OR.JZERO.LT.4) JZERO=2
   63         PRINT 905
   67         PRINT 903
   76         DO 10 I=1,51
  103         IF ( I.NE.IZERO) GO TO 16
  104         DO 14 J=1,105
  112   14    IGRID(J)=PLUS
  113         GO TO 15
  117   16    DO 11 J=1,105
  125   11    IGRID(J)=BLANK
  132   15    IGRID(JZERO)=PLUS
  133         IGRID(104)=DOT
  136         IGRID(2)=DOT
  137         DO 12 K=1,NPTS
  140         ITEST =(YMAX-Y(K))/YINCR+1.5
  144         IF(ITEST .NE.I) GO TO 12
  146         J=103.5-(XMAX-X(K))/XINCR
  152         IF(J.GT.103)J=105
  156         IF(J.LT.3) J=1
  162         IGRID(J)=STAR
  164   12    CONTINUE
  167         IF(MOD(I,10).EQ.1) GO TO 13
  174         PRINT 901,IGRID
  201         GO TO 10
  205   13    YAXIS=YMAX-(I-1)*YINCR
  211         IF(ABS(YAXIS).LT.YAXMIN) YAXIS=0.
  216         PRINT 902,YAXIS,(IGRID(J),J=1,105)
```

```
 10     CONTINUE
        PRINT 903
        PRINT 905
        DO 20 M=1,11
        XAXIS(M)=XMAX-XINCR*(FLOAT(11-M))*10.0
        IF(ABS(XAXIS(M)).LT.XAXMIN)XAXIS(M)=0.
 20     CONTINUE
        PRINT 904,XAXIS,NPTS
        RETURN
 800    PRINT 9800
        CALL EXIT
        END
```

PLSCAL

```
      SUBROUTINE PLSCAL(V,VMAX,VINCR,NPTS,NDIVIS)
C
C    SCALING PROGRAM FOR USE WITH PPNPLT    M.S.ITZKOWITZ  MAY,1967
C  THIS VERSION ADJUSTS THE FULL SCALE TO 2.5,5.0, OR 10. TIMES 10**N
C  AND ADJUSTS THE MAXIMUM POINT TO AN INTEGER MULTIPLE OF 5*VINCR
C
      DIMENSION V(NPTS)
C
      VMIN=V(1)
      VMAX=V(1)
      DO 10 I=1,NPTS
      IF(V(I).LT.VMIN) VMIN=V(I)
      IF(V(I).GT.VMAX) VMAX=V(I)
      QRANGE=VMAX-VMIN
   10 CONTINUE
      IF(QRANGE.EQ.0.) GO TO 8000
      QRANGE=0.4342944*ALOG(QRANGE)
      IF(QRANGE)20,20,30
   30 IRANGE=QRANGE
      GO TO 40
   20 IRANGE=-QRANGE
      IRANGE=-IRANGE-1
   40 QRANGE=QRANGE-FLOAT(IRANGE)
      RANGE=10.**QRANGE
C
C   RANGE IS BETWEEN 1.0 AND 10.0
C
   43 IF(RANGE.GT.2.5) GO TO 41
      RANGE=2.5
      GO TO 50
   41 IF(RANGE.GT.5.0) GO TO 42
      RANGE=5.0
      GO TO 50
   42 RANGE=10.0
   50 TRANGE=RANGE*(10.**IRANGE)
C
C   TRANGE IS NOW 2.5,5.0, OR 10.0 TIMES A POWER OF TEN
C
      VINCR=TRANGE/FLOAT(NDIVIS)
      IF(VMAX)51,51,52
   52 IMAX=VMAX/(5.0*VINCR)
      XMAX=5.0*VINCR*FLOAT(IMAX+1)
      GO TO 53
   51 IMAX=-VMAX/(5.0*VINCR)
      XMAX=5.0*VINCR*FLOAT(-IMAX+1)
   53 IF(VMIN.GT.XMAX-TRANGE) GO TO 100
      RANGE=RANGE*2.0
      IF(RANGE-10.) 43,43,54
   54 RANGE=RANGE/10.
      IRANGE=IRANGE+1
      GO TO 43
  100 VMAX=XMAX
      VMIN=XMAX-TRANGE
      RETURN
 8000 PRINT 9800
 9800 FORMAT(45H1PLSCAL CALLED TO SCALE ARRAY WITH ZERO RANGE)
      CALL EXIT
      END
```

PSIC VERSUS FILM THICKNESS
PHI = 75.00 N = 1.0000 WAVELENGTH = 5461 A NM - IKM = .
NF - IKF = 2.7500 - I .1950



DELC VERSUS FILM THICKNESS
PHI = 75.00 N = 1.0000 WAVELENGTH = 5461 A NM - IKM = .
NF - IKF = 2.7500 - I .1950

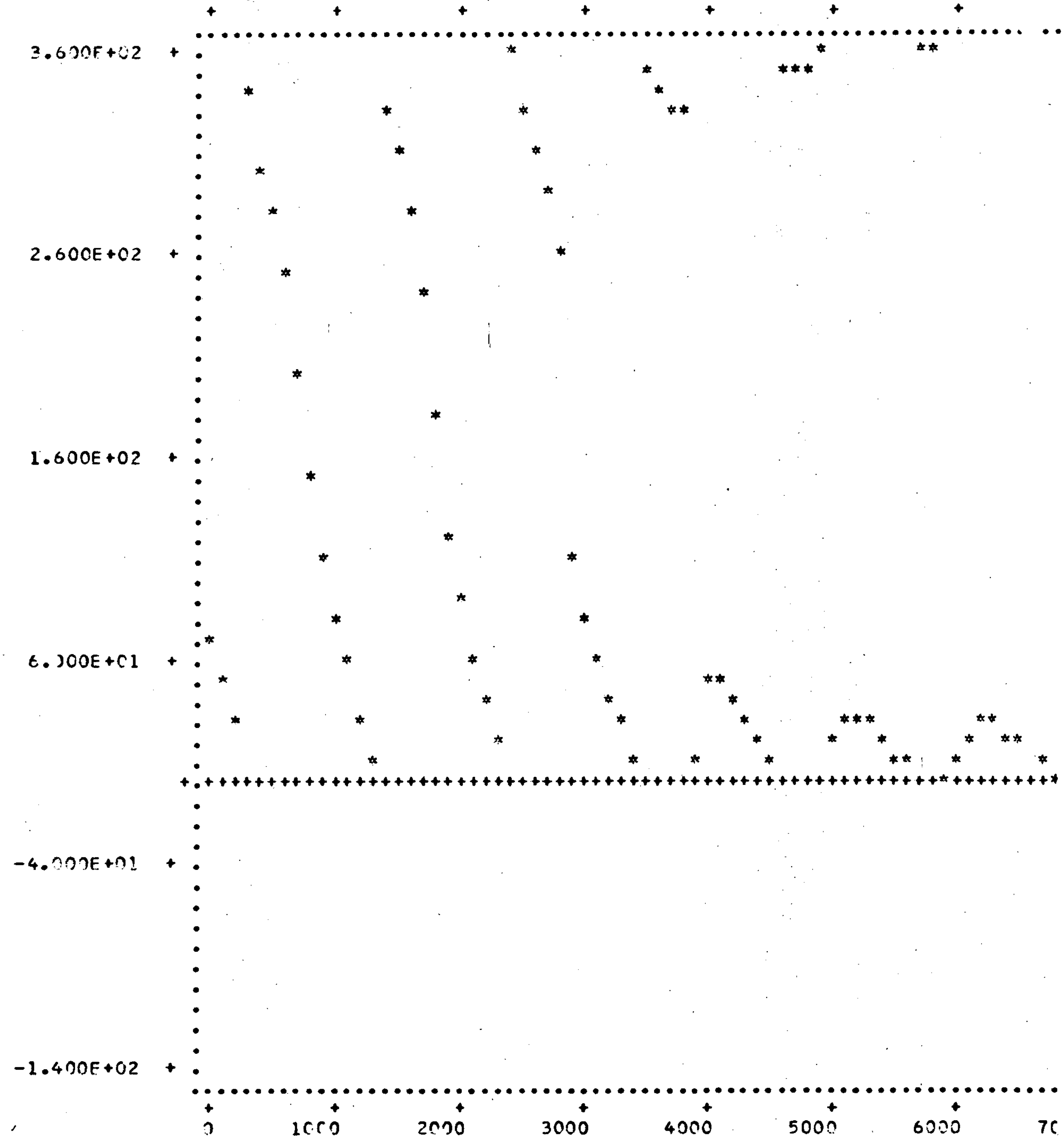


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Table I. Derivation of ψ and Δ from ellipsometer azimuths.

Zone	Range of Polarizer Transmission Azimuth p	Compensator Fast Axis Azimuth q	Range of Analyzer Transmission Azimuth a	ψ	Δ
A-1	0-45	45	90-180	180-a	90-2p
A-2	45-90	135	90-180	180-a	2p-90
A-3	90-135	45	0-90	a	270-2p
A-4	135-180	135	0-90	a	2p-270
B-1	0-45	135	0-90	a	90+2p
B-2	45-90	45	0-90	a	270-2p
B-3	90-135	135	90-180	180-a	2p-90
B-4	135-180	45	90-180	180-a	450-2p
C-1	0-45	45	0-90	a	270-2p
C-2	45-90	135	0-90	a	90+2p
C-3	90-135	45	90-180	180-a	450-2p
C-4	135-180	135	90-180	180-a	2p-90
D-1	0-45	135	90-180	180-a	270-2p
D-2	45-90	45	90-180	180-a	450-2p
D-3	90-135	135	0-90	a	90+2p
D-4	135-180	45	0-90	a	630-2p

Table II. Fortran functions used in the programs.

Name	Evaluates	Converts
CSQRT (C)	$\sqrt{C}$	complex to complex
CEXP (C)	e^{c}	complex to complex
CABS (C)	$\|C\|$	complex to real
AIMAG (C)	finds the imaginary part of C	complex to real
REAL (C)	finds the real part of C	complex to real
COX (X)	cosX	real to real
SIN (X)	sinX	real to real
ATAN (X)	$\tan^{-1}X$	real to real
ATAN2 (X,Y)	$\tan^{-1}(x/y)$	real to real
ABS (X)	$\|X\|$	real to real
CMPLX (A,B)	constructs A+iB from A,B	real to complex

If C is complex, A, B, X, Y are real.