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FORTTRAN II COMPUTER PROGRAM
FOR
ANALYSIS OF ELLIPSOMETRIC DATA

THE DOW CHEMICAL COMPANY
ROCKY FLATS DIVISION
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U.S. ATOMIC ENERGY COMMISSION
CONTRACT AT(29-1)-1106

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FORTRAN II COMPUTER PROGRAM FOR ANALYSIS OF ELLIPSOMETRIC DATA

Abstract. An accurate and time-saving procedure has been developed for the analysis of ellipsometric data related to studies of thin film formations on metal surfaces. In processing the theoretical data necessary for these studies, the margin of accuracy attained was considered sufficient. In comparing test data with work done in these areas by the recognized efforts of R. J. Archer and F. L. McCrackin, the results differed by 0.02 percent.

Since data to be processed are extensive and contain complex formulas requiring reduction to simplified interpretive solutions, accurate analyses are in demand. To date, results obtained with digital computers have offered considerable advantages over linear approximations or other solutions. Thus, a procedure was initiated utilizing a Fortran II language system and programming an ASI 210 digital computer to perform the evaluation operations. The limited memory size of the available computer however made it necessary to prepare the program, or sequence of instructions, in a series of four functional units or "links." Details are given of the program in the appendices.

INTRODUCTION

In studies of thin film formations on metal surfaces, considerable amounts of data are collected. Processing the data, solving the many related complex formulas, and interpreting the final results require tedious and time-consuming efforts. To simplify procedures in the analysis of ellipsometric data, a functional Fortran II language system was developed for use in an ASI 210 digital computer. Since the available computer was limited as to memory capacity, it had to be programmed to perform a series of operations in fixed sequences of four functional units or "links." Essentially the machine performs operations as specified by input data read into the memory portion of the machine.

Although other published works in the field of ellipsometry are available,^{1,2} analyzing them with their many variations under the 210 digital computer would have

required major modifications. Thus, the procedures described are valid only for analysis work when performed with a 210 digital computer programmed under the Fortran II language system. The details which follow do not relate to the theory of ellipsometric operations, but rather to a method for analysis of ellipsometric data. Basically, an understanding of the programming procedures will be helpful in guiding others to set up systems in computer machines for making interpretations of related comprehensive data.

DISCUSSION

Basis of Ellipsometric Theory: In studies^{3,4} of film formations, the data needed to relate the index of refraction and thickness of a thin film deposited either by metal evaporation or grown by oxide formation on a substrate are processed by the computer. Involved in the study of ellipsometry are the concepts of light rays and what happens to them while passing from one medium to another of different density.

To follow the procedures devised and understand the derived equations, a review will be helpful of Figure 1, together with definitions of symbols used throughout the report.

Calculations: The purpose of the computer program was devised to provide a means of generating the theoretical ψ or Δ curves. The experimentally *observed* quantities designated as alpha (α) and gamma (γ) are used to calculate the two quantities psi (ψ) and delta (Δ). The values of the latter two quantities are used to plot a Δ versus ψ curve. Each point on the curve represents a film thickness, and the shape of the curve determines the film's index of refraction.

The experimentally *obtained* ψ or Δ curves are then compared with a family of theoretical ψ or Δ curves which form independent of the experimental parameters and are plotted by calculating values of ψ and Δ over a range of values of film thickness "d" for various fixed values of $\hat{n}_2$. The member of this family which

¹F. L. McCrackin and J. P. Colson. *A Fortran Program for Analysis of Ellipsometer Measurements and Calculation of Reflection Coefficients from Thin Films*. Technical Note 242. U.S. Department of Commerce, Washington, D. C. 1964.

²Paul Theroux and R. C. Plumb. *Computer Program Available for Thin Film Studies Using Elliptically Polarized Light*. Journal of the Optical Society of America, 53:1451. December 1963.

³E. Passaglia, R. R. Stromberg, and J. Kruger, Editors. *Ellipsometry in the Measurement of Surfaces and Thin Films*. Miscellaneous Publication 256. U. S. Department of Commerce, National Bureau of Standards, Washington, D. C. 1964.

⁴D. T. Larson and N. W. Taylor. *Ellipsometer Studies on the Cleaning and Oxidation of Uranium*. RFP-674. Dow Chemical Company, Golden, Colorado. 1966.

FIGURE 1. Refraction of light from a film-covered surface.

Definitions

1. Medium 1 – The medium above a film.
2. Medium 2 – The film on the metal substrate.
3. Medium 3 – Metal substrate.
4. Interface 1 – The interface (surface) between the medium above the film and the film.
5. Interface 2 – The interface (surface) of the film and the substrate surface.
6. n_1 – Index of refraction of the medium above the film.
7. ϕ_1 – Angle of incidence (phi) of the ray at Interface 1.
8. n_2 – Index of refraction of the film.
9. ϕ_2 – Angle of refraction (phi) at Interface 1 or angle of incidence at Interface 2.
10. n_3 – Index of refraction of the metal substrate.
11. ϕ_3 – Angle of refraction (phi) of the ray at Interface 2.
12. λ – Wave length of the monochromatic light used. (Lambda)
13. ω – Phase change (omega) caused by quarter-wave plate in the ellipsometer.
14. ' – A single prime (') designates a parameter pertaining to a "clean" surface.
15. ^ – Indicates complex quantities.
16. α, γ – Experimental parameters (alpha and gamma) measured by the ellipsometer indicating the condition of a surface.
17. β_p – Phase angle (beta) of the component of the electric vector oscillating in the plane of incidence.
18. β_n – Phase angle (beta) of the component of the electric vector oscillating normal to the plane of incidence.
19. A_p – Amplitude of the component of the electric vector oscillating in the plane of incidence.
20. A_n – Amplitude of the component of the electric vector oscillating normal to the plane of incidence.
21. $\psi = \frac{\text{Arctan } (A_p/A_n) \text{ (reflected)}}{\text{Arctan } (A_p/A_n) \text{ (incident)}}$
22. $\Delta = [\beta_p - \beta_n \text{ (reflected)}] - [\beta_p - \beta_n \text{ (incident)}]$
23. d – Represents film thickness.
24. N, K – Factors used for calculation of optical constants of a clean metal surface.

*NOTE: Definitions taken from R. J. Archer, *Determinations of the Properties of Film on Silicon by the Method of Ellipsometry*. Journal of the Optical Society of America, 52:970. September 1962.

best fits the experimental ψ or Δ curve determines the index of refraction of the experimental film. By correlating the value of film thickness on the theoretical curve to time on the experimental curve, the film thickness--as a function of time--can be determined. Using Equations 1 and 2, the experimental ψ and Δ parameters can be calculated.⁵

$$\cos 2\psi = (\cos 2\gamma \cos 2\alpha) (1 - \cos \omega \tan 2\alpha \tan 2\gamma) \quad (1)$$

$$\cos \Delta = \frac{(\cos 2\gamma \cos 2\alpha) (\tan 2\alpha + \cos \omega \tan 2\gamma)}{\sin 2\psi} \quad (2)$$

The theoretical ψ and Δ parameters are calculated using the following method. First, calculate $\hat{n}_3$, the index of refraction of the substrate. This is done by using the experimental values α' and γ' for the "clean" surface to calculate ψ' and Δ' by Equations 1 and 2.

The calculated values of ψ' and Δ' are used to determine two additional quantities N and K defined by:⁶

$$N^2 = (n_1)^2 \sin^2 \phi_1 \left[1 + \frac{\tan^2 \phi_1 \cos^2 (2\psi')}{(1 + \sin 2\psi' \cos \Delta')^2} \right] \quad (3)$$

$$K = \frac{n_1 \tan \phi_1 \sin \phi_1 \sin 2\psi' \sin \Delta'}{(1 + \sin 2\psi' \cos \Delta')} \quad (4)$$

The angle ϕ_3' is defined as the angle of refraction in the substrate when the substrate has no film on it. The angle may be calculated from the equation:

$$\cos^2 \phi_3' = 1 - \left(\frac{n_1^2 \sin^2 \phi_1}{N^2} \right) \quad (5)$$

The index of refraction of the substrate is found by calculating the equation:

$$\hat{n}_3^2 = (N^2 - K^2) - (2iNK \cos \phi_3') \quad (6)$$

Once $\hat{n}_3$ is known, the following equations are solved to get ψ and Δ .⁷ From Snell's Law, it is possible to calculate the angles $\hat{\phi}_2$ and $\hat{\phi}_3$ for various selected values of $\hat{n}_2$:

$$n_1 \sin \phi_1 = \hat{n}_2 \sin \hat{\phi}_2 \quad (7)$$

$$\hat{n}_2 \sin \hat{\phi}_2 = \hat{n}_3 \sin \hat{\phi}_3 \quad (8)$$

The equations for the Fresnel coefficients are used to provide the reflection coefficients for polarized light reflected from an interface. The equations are:

$$\hat{r}_{ab}^p = \frac{(\hat{n}_b \cos \hat{\phi}_a) - (\hat{n}_a \cos \hat{\phi}_b)}{(\hat{n}_b \cos \hat{\phi}_a) + (\hat{n}_a \cos \hat{\phi}_b)} \quad (9)$$

$$\hat{r}_{ab}^n = \frac{(\hat{n}_a \cos \hat{\phi}_a) - (\hat{n}_b \cos \hat{\phi}_b)}{(\hat{n}_a \cos \hat{\phi}_a) + (\hat{n}_b \cos \hat{\phi}_b)} \quad (10)$$

Relative to Equations (9) and (10), the notations designate the following:

$\hat{r}_{ab}^p$ and $\hat{r}_{ab}^n$ — Fresnel coefficients for light being refracted at the interface between mediums "a" and "b."

"p" — Superscript refers to that component of the electric vector oscillating in the plane of incidence.

"n" — Superscript refers to that component of the electric vector oscillating normal to the plane of incidence.

$\hat{\phi}_a$ and $\hat{n}_a$ — Represent, respectively, the angle of incidence of the ray at the interface and the index of refraction of medium "a."

$\hat{\phi}_b$ and $\hat{n}_b$ — Represent, respectively, the angle of refraction of the ray at the interface and the index of refraction of medium "b."

To understand the equations solved for values of $\hat{r}_{ab}^p$ and $\hat{r}_{ab}^n$, consider the following:

1. $b = a + 1$
 $a = 1, 2$
2. The subscripts 1, 2, and 3 represent the mediums above the film, the film, and the metal substrate, respectively.
3. The following are, in general, complex:
 $\hat{r}_{ab}^p$; $\hat{r}_{ab}^n$; $\hat{n}_2$;
 $\hat{n}_3$; $\hat{\phi}_2$; and $\hat{\phi}_3$
4. The notation "i" represents an imaginary number.

After $\hat{r}_{ab}^p$ and $\hat{r}_{ab}^n$ are calculated for all values of "a" and "b," use the Drude equations for calculating the reflection coefficients for a film-covered surface:

$$\hat{R}_p = \frac{\hat{r}_{12}^p + \hat{r}_{23}^p \exp(-2i\delta)}{1 + \hat{r}_{12}^p \hat{r}_{23}^p \exp(-2i\delta)} \quad (11)$$

$$\hat{R}_n = \frac{\hat{r}_{12}^n + \hat{r}_{23}^n \exp(-2i\delta)}{1 + \hat{r}_{12}^n \hat{r}_{23}^n \exp(-2i\delta)} \quad (12)$$

In order to complete the determinations of $\hat{R}_p$ and $\hat{R}_n$, it is necessary to calculate the value of δ . This is done using the following formula where "d" represents the film thickness and is selectively varied over a specified range:

$$\delta = \frac{2\pi \hat{n}_2 \cos \hat{\phi}_2 d}{\lambda} \quad (13)$$

⁵R. C. Plumb. *Analysis of Elliptically Polarized Light*. Journal of the Optical Society of America, 50:892. September 1960.

⁶A. Vasicek. "Optical Study of a Thin Absorbing Film on a Metal Surface." *Ellipsometry in the Measurement of Surfaces and Thin Films*. Loc. cit., pp. 25-39.

⁷Paul Theroux and R. C. Plumb. Loc. cit., p. 1451.

The values of the reflection coefficients $\hat{R}_p$ and $\hat{R}_n$ are used in the following expression for the determinations of $\tan \psi$ and Δ :

$$\tan \psi \exp(i\Delta) = \frac{\hat{R}_p}{\hat{R}_n} \quad (14)$$

Thus by selectively varying "d" over a specified range for each value of $\hat{n}_2$ chosen, the required family of theoretical ψ or Δ curves are generated.

$\tan \psi$ and Δ represent, respectively, the relative attenuation and the difference of phase shifts of the reflected polarized light for the components of the electric vector oscillating in the plane of incidence and normal to the plane.

Programing the Data: The program was prepared to process, continuously and automatically, as many independent sets of input data as could be loaded on the tape reader of the computer.

The tape device permits punching of "input" data which are in turn yielded by the computer as punched "output" data easily interpreted. For example, meaningful results can be obtained by starting at any of the following locations:

1. Input of α' , γ' , and ω
2. Input of ψ' and Δ'
3. Input of $\hat{n}_3$

There is the additional option of starting with an approximate correct value of $\hat{n}_3$ and then trying to refine the approximation. When this operation is completed, the program structure permits an experimenter to determine the following information by checking the output data:

- a. The possibility or not of refining the approximations.
- b. If no possibility, which part of $\hat{n}_3$, real or imaginary, caused the computer to terminate the refinement process.
- c. The number of cycles the computer made while trying to refine the approximation.

Flow Diagrams for Computer Program: The magnitude of the problems to be solved and the limited memory of the ASI-210 digital computer made it necessary to program the data in a series of four units or "links." The flow diagrams attached as appendices to the report show the full details relating to problem solutions.

Specifically, *Appendix A* contains flow diagrams showing how the four links of the program are related. *Appendices B, C, D, and E*, respectively, show flow diagrams for each of the four links:

Links 1, 2, 3, and 4.

Complete lists of the Fortran II language system used to solve the various problems are illustrated in *Appendices F, G, H, and I*.

Attached also is *Appendix J*, a Glossary, containing a list of problem variables and corresponding names to facilitate an understanding of computer program uses.

CONCLUSIONS

Through computer programing, considerable time, effort, and many man-hours of computation can be saved in the analysis of ellipsometric data in studies of thin film formations. Although the report describes certain limitations of the ASI-210 digital computer, there is no question as to the advantages derived from the easy solutions of the comprehensive data involved. The yield or results give valid and accurate data in less time than what can be achieved through linear approximations or other known solutions.

Data Comparisons: Comparisons of the data in this program with those obtained by R. J. Archer (see reference note under Figure 1) for values of real n_2 indicate a relative average variation of 0.02 percent, which is of sufficient accuracy.

Data, using complex $\hat{n}_2$ and supplied through personal discussions with F. L. McCrackin, agreed with results obtained.

Appendix A. MASTER FLOW DIAGRAM OF LINKS.

►NOTE: The variable names indicated in the flow chart are marked with a bullet (►) at the far left of the notations for the computer program sheets identified as Appendices G and H.

Appendix B. FLOW DIAGRAM OF LINK 1.

Appendix C. FLOW DIAGRAM OF LINK 2.

Appendix D. FLOW DIAGRAM OF LINK 3.

NOTE: The variable R_n is indicated as R_M in the Appendix H.

Appendix E. FLOW DIAGRAM OF LINK 4.

Appendix E. FLOW DIAGRAM OF LINK 4. (Continued)

Appendix E. FLOW DIAGRAM OF LINK 4. (Concluded)

Appendix F. COMPUTER PROGRAM FOR LINK 1.

```

LINK1,1
DIMENSION EN21(10),EN22(10),D(10)
COMMON EN21,EN22,D,EN1,PH11,ELAMDA,TOL,ISTOP,TANPSI
COMMON IPICK,IPATH,IGO,IBEGIN,NN,M,MM
COMMON PSIP,DELP,ALPHAP,GAMMAP,OMEGA,S2PN12,PSI
COMMON EN31,EN32,SINP31,COSP31,SNHP32,COHP32,I,J,K,DEL
COMMON LOOPS,EN311,EN321,DIFF1,DIFF2,DIFF11,DIFF21
1  FORMAT(12)
2  FORMAT(F5.2)
3  FORMAT(F7.2)
4  FORMAT(F4.1)
  READ1,IPICK
  READ1,IPATH
  IGO=0
  IBEGIN=0
  READ1,NN
  READ1,M
  READ1,MM
  DO 100 I=1,M
100  READ2,EN21(I)
    CONTINUE
    DO 102 J=1,MM
102  READ2,EN22(J)
    CONTINUE
    DO 104 K=1,NN
104  READ3,D(K)
    CONTINUE
    READ4,EN1
    READ4,PH11
    READ3,ELAMDA
    PH11=PH11/57.29578
    IF(IPATH)106,108,108
106  READ2,TOL
108  CALL CHAINF(2,1)
  END
EOF

```


Appendix G. COMPUTER PROGRAM FOR LINK 2.

```

LINK2,1
DIMENSION EN21(10),EN22(10),D(10)
COMMON EN21,EN22,D,EN1,PHI1,ELAMDA,TOL,ISTOP,TANPSI
COMMON IPICK,IPATH,IGO,IBEGIN,NN,M,MM
COMMON PSIP,DELP,ALPHAP,GAMMAP,OMEGA,S2PN12,PSI
COMMON EN31,EN32,SINP31,COSP31,SNHP32,COHP32,I,J,K,DEL
COMMON LOOPS,EN311,EN321,DIFF1,DIFF2,DIFF11,DIFF21
1  FORMAT (F8.3)
2  FORMAT (F5.1)
3  FORMAT (F6.1)
4  FORMAT (F7.4)
   IF (IBEGIN)112,100,112
100 IF(IPICK)102,104,114
102 READ1,PSIP
   READ1,DELP
   PSIP=PSIP/57.29578
   DELP=DELP/57.29578
   GO TO 112
104 READ2,ALPHAP
   READ2,GAMMAP
   READ3,OMEGA
   ALPHAP=ALPHAP/57.29578
   GAMMAP=GAMMAP/57.29578
   OMEGA=OMEGA/57.29578
   COS2SP=COSF(2.0*GAMMAP)*COSF(2.0*ALPHAP)*(1.0-COSF(OMEGA)*
1(SINF(2.0*ALPHAP)/COSF(2.0*ALPHAP))*(SINF(2.0*GAMMAP)/COSF(2.0*
2GAMMAP)))
   SIN2SP=SQRTF(1.0-COS2SP**2)
   IF(COS2SP)106,108,108
106 ►PSIP=1.57079+ATANF(SIN2SP/COS2SP)/2.0
   GO TO 110
108 ►PSIP=ATANF(SIN2SP/COS2SP)/2.0
110 COSDIP=1.0/SIN2SP*COSF(2.0*GAMMAP)*COSF(2.0*ALPHAP)*
1(SINF(2.0*ALPHAP)/COSF(2.0*ALPHAP))+COSF(OMEGA)*(SINF(2.0*
2GAMMAP)/COSF(2.0*GAMMAP)))
   SINDIP=SQRTF(1.0-COSDIP**2)
   IF(COSDIP)109,111,111
109 ►DELP=3.14159+ATANF(SINDIP/COSDIP)
   GO TO 112

```

►NOTE: The variable names indicated in the flow chart are marked with a bullet (►) at the far left of the notations for the computer program sheets identified as Appendices G and H.

Appendix G. COMPUTER PROGRAM FOR LINK 2. (Concluded)

```

111  ► DELP=3.14159-ATANF(SIND1P/COSD1P)
112  ► S2PN12=EN1**2*SINF(PH11)**2
      EN2=S2PN12*(1.0+(SINF(PH11)/COSF(PH11))**2*(COSF(2.0*PSIP)**2)
      1/(1.0+SINF(2.0*PSIP)*COSF(DELP))**2)
      ► EN=SQRTF(EN2)
      ► EK=EN1*(SINF(PH11)/COSF(PH11))*SINF(PH11)*SINF(2.0*PSIP)*
      1SINF(DELP)/(1.0+SINF(2.0*PSIP)*COSF(DELP))
      ► COSP3P=SQRTF(1.0-S2PN12/EN2)
      EN312=((EN2-EK**2)+SQRTF((EN2-EK**2)**2+4.0*EN2*EK**2
      1*COSP3P**2))/2.0
      ► EN31=SQRTF(EN312)
      EN322=(-(EN2-EK**2)+SQRTF((EN2-EK**2)**2+4.0*EN2*EK**2
      1*COSP3P**2))/2.0
      ► EN32=SQRTF(EN322)
      GO TO 116
114  READ4,EN31
      READ4,EN32
      EN312=EN31**2
      EN322=EN32**2
      S2PN12=EN1**2*SINF(PH11)**2
116  ► SINP31=SQRTF(1.0/2.0+S2PN12/(2.0*(EN312+EN322))-SQRTF(
      11.0/4.01(1.0/2.0*S2PN12*(EN322-EN312))/((EN312+EN322)**2)+
      2S2PN12**2/(4.0*(EN312+EN322)**2)))
      COSP31=SQRTF(1.0-SINP31**2)
      ► SNHP32=SQRTF(S2PN12/(2.0*(EN312+EN322))-1.0/2.0+SQRTF(
      11.0/4.0+(1.0/2.0*S2PN12*(EN322-EN312)/(EN312+EN322)**2)+
      2S2PN12**2/(4.0*(EN312+EN322)**2)))
      COHP32=SQRTF(1.0+SNHP32**2)
      I=1
      J=1
      K=1
      CALL CHAINF(3,1)
      END
      EOF

```

►NOTE: The variable names indicated in the flow chart are marked with a bullet (►) at the far left of the notations for the computer program sheets identified as Appendices G and H.

Appendix H. COMPUTER PROGRAM FOR LINK 3.

```

LINK3,1
DIMENSION EN21(10),EN22(10),D(10)
COMMON EN21,EN22,D,EN1,PHI1,ELAMDA,TOL,ISTOP,TANPS;
COMMON IPICK,IPATH,IGO,IBEGIN,NN,M,MM
COMMON PSIP,DELP,ALPHAP,GAMMAP,OMEGA,S2PN12,PS;
COMMON EN31,EN32,SINP31,COSP31,SNHP32,COHP32,I,J,K,DEL
COMMON LOOPS,EN311,EN321,DIFF1,DIFF2,DIFF11,DIFF21
200 SUM2N2=(EN21(I)**2)+(EN22(J)**2)
    DIF2N2=(EN22(J)**2)-(EN21(I)**2)
    ▶SINP21=SQRTF((1.0/2.0)+(S2PN12/(2.0*SUM2N2))-SQRTF((1.0/4.0)+
    1(S2PN12/2.0)*(DIF2N2/(SUM2N2**2))+((S2PN12**2)/(4.0*(SUM2N2**2)
    2))))
    COSP21=SQRTF(1.0-(SINP21**2))
    IF(EN22(J)-0.000)220,220,210
220 ▶SNHP22=0.000
    GO TO 230
210 ▶SNHP22=SQRTF((S2PN12/(2.0*SUM2N2))-(1.0/2.0)+SQRTF((1.0/4.0)+
    1(S2PN12/2.0)*(DIF2N2/(SUM2N2**2))+((S2PN12**2)/(4.0*
    2(SUM2N2**2)))))
230 COHP22=SQRTF(1.0+(SNHP22**2))
    RPHI21=COSP21*COHP22
    CPHI22=+(SINP21*SNHP22)
    RPHI31=COSP31*COHP32
    CPHI32=+(SINP31*SNHP32)
    ▶DELTA1=(2.*3.14159*D(K)/ELAMDA)*((EN21(I)*RPHI21)-(EN22(J)*CPHI22
    1))
    ▶DELTA2=-((2.0*3.14159*D(K))/ELAMDA)*((EN21(I)*CPHI22)+(EN22(J)*
    1RPHI21))
    A12P=(EN21(I)*COSF(PHI1))-(EN1*RPHI21)
    B12P=(EN21(I)*COSF(PHI1))+(EN1*RPHI21)
    D12P=(EN1*CPHI22)-(EN22(J)*COSF(PHI1))
    E12P=(EN1*CPHI22)+(EN22(J)*COSF(PHI1))
    ▶R12P=((A12P*B12P)-(D12P*E12P))/((B12P**2)+(E12P**2))
    C12P=((A12P*E12P)+(B12P*D12P))/((B12P**2)+(E12P**2))
    A12N=(EN1*COSF(PHI1))-(EN21(I)*RPHI21)+(EN22(J)*CPHI22)
    B12N=(EN1*COSF(PHI1))+(EN21(I)*RPHI21)-(EN22(J)*CPHI22)
    D12N=(EN21(I)*CPHI22)+(EN22(J)*RPHI21)
    ▶R12N=((A12N*B12N)-(D12N**2))/((B12N**2)+(D12N**2))
    C12N=((A12N*D12N)+(B12N*D12N))/((B12N**2)+(D12N**2))
    A23P=(EN31*RPHI21)-(EN32*CPHI22)-(EN21(I)*RPHI31)+(EN22(J)*
    1CPHI32)
    B23P=(EN31*RPHI21)-(EN32*CPHI22)+(EN21(I)*RPHI31)-(EN22(J)
    1*CPHI32)
    D23P=(EN31*CPHI22)+(EN32*RPHI21)-(EN21(I)*CPHI32)-(EN22(J)
    1*RPHI31)
    E23P=(EN31*CPHI22)+(EN32*RPHI21)+(EN21(I)*CPHI32)+(EN22(J)
    1*RPHI31)
    ▶R23P=((A23P*B23P)+(D23P*E23P))/((B23P**2)+(E23P**2))
    C23P=((A23P*E23P)-(B23P*D23P))/((B23P**2)+(E23P**2))
    A23N=(EN21(I)*RPHI21)-(EN22(J)*CPHI22)-(EN31*RPHI31)+(EN32*
    1CPHI32)
    B23N=(EN21(I)*RPHI21)-(EN22(J)*CPHI22)+(EN31*RPHI31)-(EN32*
    1CPHI32)

```

▶NOTE 1: The variable names indicated in the flow chart are marked with a bullet (▶) at the far left of the notations for the computer program sheets identified as Appendices G and H.

NOTE 2: The notation RM in the computer program is indicated as Rn in the flow diagram.

Appendix H. COMPUTER PROGRAM FOR LINK 3. (Concluded)

```

D23N=(EN21(I)*CPH122)+(EN22(J)*RPH121)-(EN31*CPH132)-(EN32*
1RPH131)
E23N=(EN21(I)*CPH122)+(EN22(J)*RPH121)+(EN31*CPH132)+(EN32*
1RPH131)
►R23N=((A23N*B23N)+(D23N*E23N))/((B23N**2)+(E23N**2))
C23N=((A23N*E23N)-(B23N*D23N))/((B23N**2)+(E23N**2))
AP=R12P+((R23P*COSF(2.0*DELTA1))+(C23P*SINF(2.0*DELTA1)))*
1EXPF(2.0*DELTA2)
BP=1.0+((R12P*R23P*COSF(2.0*DELTA1))+(R12P*C23P*SINF(2.0*DELTA1)
1)-(C12P*C23P*COSF(2.0*DELTA1))+(C12P*R23P*SINF(2.0*DELTA1)))*
2EXPF(2.0*DELTA2)
DP=C12P+((C23P*COSF(2.0*DELTA1))-(R23P*SINF(2.0*DELTA1)))*
1EXPF(2.0*DELTA2)
EP=((C12P*R23P*COSF(2.0*DELTA1))+(C12P*C23P*SINF(2.0*DELTA1))+
1(R12P*C23P*COSF(2.0*DELTA1))-(R12P*R23P*SINF(2.0*DELTA1)))*
2EXPF(2.0*DELTA2)
►RP=((AP*BP)+(DP*EP))/((BP**2)+(EP**2))
CP=((DP*BP)-(AP*EP))/((BP**2)+(EP**2))
AM=R12N+((R23N*COSF(2.0*DELTA1))+(C23N*SINF(2.0*DELTA1)))*
1EXPF(2.0*DELTA2)
BM=1.0+((R12N*R23N*COSF(2.0*DELTA1))+(R12N*C23N*SINF(2.0*DELTA1)
1)-(C12N*C23N*COSF(2.0*DELTA1))+(C12N*R23N*SINF(2.0*DELTA1)))*
2EXPF(2.0*DELTA2)
DM=C12N+((C23N*COSF(2.0*DELTA1))-(R23N*SINF(2.0*DELTA1)))*
1EXPF(2.0*DELTA2)
EM=((C12N*R23N*COSF(2.0*DELTA1))+(C12N*C23N*SINF(2.0*DELTA1))+
1(R12N*C23N*COSF(2.0*DELTA1))-(R12N*R23N*SINF(2.0*DELTA1)))*
2EXPF(2.0*DELTA2)
►RM=((AM*BM)+(DM*EM))/((BM**2)+(EM**2))
CM=((DM*BM)-(AM*EM))/((BM**2)+(EM**2))
TANPSI=SQRTF(((RP*RM)+(CP*CM)**2)+(((RM*CP)-(RP*CM))**2))/
1((RM**2)+(CM**2))
►PSI=ATANF(TANPSI)*57.29578
SINDEL=((RM*CP)-(RP*CM))/SQRTF(((RP*RM)+(CP*CM)**2)+
1((RM*CP)-(RP*CM))**2))
COSDEL=(RP*RM+CP*CM)/SQRTF((RP*RM+CP*CM)**2+
1(RM*CP-RP*CM)**2)
300 IF(SINDEL)310,300,300
302 IF(COSDEL)304,306,302
304 ►DEL=57.29578*ATANF(SINDEL/COSDEL)
GO TO 333
306 DEL=57.29578*(3.14159-ATANF(SINDEL/(-COSDEL)))
GO TO 333
310 DEL=90.0
GO TO 333
312 IF(COSDEL)314,316,312
314 DEL=57.29578*(6.28318-ATANF((-SINDEL)/COSDEL))
GO TO 333
316 DEL=57.29578*(3.14159+ATANF(SINDEL/COSDEL))
GO TO 333
333 DEL=270.0
CALL CHAINF(4,1)
END
EOF ►NOTE 1: The variable names indicated in the flow chart are marked with a bullet (►) at the far left
of the notations for the computer program sheets identified as Appendices G and H.
NOTE 2: The notation RM in the computer program is indicated as Rn in the flow diagram.

```

Appendix I. COMPUTER PROGRAM FOR LINK 4.

```

LINK4,1
DIMENSION EN21(10),EN22(10),D(10)
COMMON EN21,EN22,D,EN1,PHI1,ELAMDA,TOL,ISTOP,TANPSI
COMMON IPICK,IPATH,IGO,IBEGIN,NN,M,MM
COMMON PSIP,DELP,ALPHAP,GAMMAP,OMEGA,S2PN12,PSI
COMMON EN31,EN32,SINP31,COSP31,SNHP32,COHP32,I,J,K,DEL
COMMON LOOPS,EN311,EN321,DIFF1,DIFF2,DIFF11,DIFF21
1  FORMAT(4F10.5)
2  FORMAT(7H N1= 7X,F4.1)
3  FORMAT(9H PHI1= F9.1)
4  FORMAT(10H LAMBDA=F8.2)
5  FORMAT(11H ALPHAP= F7.1)
6  FORMAT(11H GAMMAP= F7.1)
7  FORMAT(11H OMEGA= F7.1)
8  FORMAT(11H PSIP= F7.1)
9  FORMAT(11H DELP= F7.1)
10 FORMAT(8H N31= F10.5)
11 FORMAT(8H N32= F10.5)
12 FORMAT(10H LOOPS= i8)
13 FORMAT(54HACCEPTABLE VALUES FOR N31 AND N32 HAVE BEEN CALCULATED)
14 FORMAT(49HAN ACCEPTABLE VALUE FOR N31 CAN NOT BE CALCULATED)
15 FORMAT(49HAN ACCEPTABLE VALUE FOR N32 CAN NOT BE CALCULATED)
16 FORMAT(1H )
17 FORMAT(2X,5H N21 3X,5H N22 3X,4H D 11H TAN(PSI)
13X,5H PSI 4X,5H DEL )
18 FORMAT(2F8.3,F7.1,F11.5,2F9.4)
   IF(IPATH)100,130,148
100  IF(IPATH+2)102,102,110
102  IPATH=-1
      LOOPS=0
104  LOOPS=LOOPS+1
      EN311=EN31
      EN321=EN32
      XPSIP=57.29578*PSIP
      XDELP=57.29578*DELP
      IF(SENSE SWITCH1)106,108
106  PUNCH1,EN31,EN32,XPSIP,XDELP
108  PSIP=PSI/57.29578
      DELP=DEL/57.29578
      IBEGIN=1
      CALLCHAINF(2,1)
110  DIFF1=EN31-EN311
      DIFF2=EN32-EN321
      IF(IGO)112,112,116
112  IGO=1
114  DIFF11=DIFF1
      DIFF21=DIFF2
      GO TO104
116  IF(ABSF(DIFF1)-TOL*EN311)126,126,118
118  IF(ABSF(DIFF1)-ABSF(DIFF11))122,120,120
120  ISTOP=22
      GOTO130

```

Appendix I. COMPUTER PROGRAM FOR LINK 4. (Concluded)

```

122 IF (ABS F(DIFF2)-ABS F(DIFF21))114,124,124
124 ISTOP=33
    GOTO130
126 IF (ABS F(DIFF2)-TOL*EN321)128,128,122
128 ISTOP=11
130 APH11=57.29578*PH11
    PUNCH2,EN1
    PUNCH3,APH11
    PUNCH4,ELAMDA
    IF (IPICK)134,132,136
132 ALPHAP=57.29578*ALPHAP
    GAMMAP=57.29578*GAMMAP
    OMEGA=57.29578*OMEGA
    PUNCH5,ALPHAP
    PUNCH6,GAMMAP
    PUNCH7,OMEGA
134 PSIP=57.29578*PSIP
    DELP=57.29578*DELP
    PUNCH8,PSIP
    PUNCH9,DELP
136 PUNCH10,EN31
    PUNCH11,EN32
    IF (IBEGIN)146,146,138
138 PUNCH12,LOOPS
    IF (ISTOP-22)140,142,144
140 PUNCH13
    GOTO146
142 PUNCH14
    GOTO146
144 PUNCH15
146 PUNCH16
    PUNCH17
    PUNCH16
    IPATH=1
148 PUNCH18,EN21(I),EN22(J),D(K),TANPSI,PSI,DEL
    IF (K-NN)150,152,152
150 K=K+1
    CALL CHA:INF(3,1)
152 K=1
    IF (J-MM)154,156,156
154 J=J+1
    CALL CHA:INF(3,1)
156 J=1
    IF (I-M)158,160,160
158 I=I+1
    CALL CHA:INF(3,1)
160 PUNCH 16
    PUNCH 16
    PUNCH 16
    CALL CHA:INF(1,1)
    END
    EOF

```


Appendix J. GLOSSARY.

PROBLEM VARIABLE	PROGRAM NAME	PROBLEM VARIABLE	PROGRAM NAME
n_1	EN1	$\sin(\hat{\phi}_3, \text{Real})$	SINP31
$\hat{n}_2, \text{Real}$	EN21	$\sinh(\hat{\phi}_3, \text{Imaginary})$	SNHP32
$\hat{n}_2, \text{Imaginary}$	EN22	$\sin(\Delta)$	SINDEL
$\hat{n}_3, \text{Real}$	EN31	$\cos(\Delta)$	COSDEL
$(\hat{n}_3, \text{Real})^2$	EN312	$\sin(\Delta')$	SIND1P
$\hat{n}_3, \text{Imaginary}$	EN32	$\cos(\Delta')$	COSD1P
$(\hat{n}_3, \text{Imaginary})^2$	EN322	$\tan(\psi)$	TANPSI
N	EN	$\sin(2\psi')$	SIN2SP
N^2	EN2	$\cos(2\psi')$	COS2SP
K	EK	$n_1^2 \sin^2(\phi_1)$	S2PN12
ϕ_1 (degrees)	APHI1	Film Thickness, "d"	D
ϕ_1	PHI1	Number of "d" values	NN(≤ 1)
α'	ALPHAP	Number of $\hat{n}_2, \text{Real}$, values	M(≤ 1)
γ'	GAMMAP	Number of $\hat{n}_2, \text{Imaginary}$, values	MM(≤ 1)
ψ'	PSIP	Previously calculated value of EN31	EN311
ψ	PSI	Previously calculated value of EN32	EN321
Δ'	DELP	EN31 - EN311	DIFF1
Δ	DEL	EN32 - EN321	DIFF2
$\hat{\delta}, \text{Real}$	DELTA1	Previous value of DIFF1	DIFF11
$\hat{\delta}, \text{Imaginary}$	DELTA2	Previous value of DIFF2	DIFF21
λ	ELAMDA	Maximum acceptable value of both	
ω	OMEGA	of the following: DIFF1/EN31	TOL
$\cos(\phi_3)$	COSP3P	DIFF2/EN32	
$\sin(\hat{\phi}_2, \text{Real})$	SINP21	Number of cycles completed in the	
$\sinh(\hat{\phi}_2, \text{Imaginary})$	SNHP22	refining process for EN31 and EN32	LOOPS