Title
COMPUTER PROGRAMS FOR ELLIPSOMETRY II

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Publication Date
1973-12-01

LBL-2517
c.2

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December 1973

Prepared for the U.S. Atomic Energy
Commission under Contract W-7405-ENG-48

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COMPUTER PROGRAMS FOR ELLIPSOMETRY II

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ABSTRACT

This report describes two additional computer programs in Fortran IV language for use in interpreting ellipsometer measurements. One program considers the case of a substrate covered with two films of different refractive index and of different thickness, the other a substrate covered with an inhonogeneous film with continuously varying refractive index, represented by multiple films of equal thickness and monotonically varying optical properties.

I. FORTRAN IV COMPUTER PROGRAM "DUALF"

This program will evaluate ellipsometer-quantities ψ and Δ of a substrate covered with two homogeneous parallel films of variable thickness[1] (Fig. 1a). It makes partial use of a previous program "LAYER", which assumes coverage by only one film, and "CMOC", which converts reflection coefficient into the complex refractive index of a bare surface.[2]

Program "DUALF" computes ψ and Δ in two steps. In the first step one assumes that the substrate (see Fig. 1b) is only covered with one film (Film 2) of thickness TI. Film 1 is assumed as the incident medium. Drude's equation[1,3] is applied to determine the complex ratio of reflection coefficients, ρ, defined as

$$\rho = \frac{r_p}{r_s}$$

with r_p as the reflection coefficient for the component parallel to the plane of incident and r_s for the component perpendicular to the plane of incidence.

Once ρ is computed, one can determine the effective complex refractive index n_s' of the combined system of substrate and Film 2 of thickness TI. This new refractive index n_s' is used in the second step as the new substrate covered with Film 1 of thickness TlI (Fig. 1c). These new data of substrate S' and Film 1 are applied to Drude's equation again to determine ρ', which can be converted to ψ and Δ, according to

$$\rho' = \tan\psi \exp(i\Delta)$$

Computations are performed by systematically combining all prescribed values of optical constants and film thicknesses for both layers with fixed properties of substrate and incident media.

This program was tested for decreasing film thickness of Film 2 (TI→0Å) and $n_2 \to n_1$ to give the same results as program "LAYER".

A. Variables Used in the Program DUALF

Name	Description
AC	Analyzer azimuth (zone A3), for dual-film system
DELC	Ellipsometric parameter Δ, for dual-film system
DT	Increment of thickness of Film 2
DTN	Increment of real part of refractive index of Film 2
DTNK	Increment of imaginary part of refractive index of Film 2
DTNK1	Increment of imaginary part of refractive index of Film 1
DTN1	Increment of real part of refractive index of Film 1
D1T	Increment of thickness of Film 1
PC	Polarizer azimuth (zone A3) for dual-film system
PHI1,PHI	Angle of incidence
PSIC	Ellipsometric parameter ψ for dual-film system
TI	Initial thickness of Film 2
TM	Final thickness of Film 2
TN1	Real part of refractive index of Film 2, initial value
TNKI	Imaginary part of refractive index of Film 2
TNKM	Imaginary part of refractive index of Film 2, final value
TNKS	Imaginary part of refractive index of substrate
TNK1I	Imaginary part of refractive index of Film 1, initial value
TNK1M	Imaginary part of refractive index of Film 1, final value
TNM	Real part of refractive index of Film 2, final value
TNO,N	Refractive index of incident medium (real)

TNS	Real part of refractive index of substrate
TN1I	Real part of refractive index of Film 1, initial value
TN1M	Real part of refractive index of Film 1, final value
T1I	Initial thickness of Film 1
T1M	Final thickness of Film 1
WL	Wavelength of light in vacuum

B. Input Format for Program DUALF

Card	1-9	10-19	20-29	30-39	40-49	50-59
1 2	Title and comments (up to 80 columns each)					
3	TNO	WL	TNS	TNKS	PHI1	
4	TNI	DTN	TNM	TNKI	DTNK	TNKM
5	TI	DT	TM			
6	TN1I	DTN1	TN1M	TNK1I	DTNK1	TNK1M
7	TI1	D1T	D1M			

These seven cards constitute a set. Any number of sets may follow. Three blank cards must follow the last set of data. The program, together with a sample of output, is reproduced below.

For zone A3, the range of data for polarizer and analyzer readings are[3]

range of polarizer transmission reading	0-45°
range of analyzer transmission reading	90-180°
compensator circle reading	135°

Azimuth readings differ from circle readings of the present ellipsometer by 90°:

P(azimuth) = P(circle reading) + 90°

A(azimuth) = A(circle reading) - 90°

DUALF

```
              PROGRAM DUALF (INPUT,OUTPUT)
        C     THIS PROGRAM CALCULATES THE ELLIPSOMETRIC PARAMETERS
        C     DELC,PSIC OF A SUBSTRATE COVERED WITH TWO FILMS.
        C     THE INCIDENT MEDIUM HAS THE REAL REFRACTIVE INDEX TNO
        C     FILM (1) HAS THE OPTICAL CONSTANTS TN1 AND TN1K WITH
        C     THICKNESS T1I TO T1M
        C     FILM (2) NEXT TO THE SUBSTRATE HAS THE OPTICAL
        C     CONSTANTS TN,TNK WITH THICKNESS TI TO TM
        C     THE COMPUTATION STARTS FROM THE BOTTOM (SUBSTRATE)
        C     AC AND PC ARE VALID FORE ZONE A3
              COMPLEX TN1,T2,S2,TN3,LN3, LN2     ,S1,T1,SC,CC,D
              COMPLEX TN2,        CPHI2, CPHI3, R1S, R1P, R2S, R2P,    RS, RP, RHO
              REAL PHI1,PHI,CP,SP,LNK,LN,L,TN,TNK,T,PSIC,DELC,DT,TM
              REAL DTNK1,TNKM,T1M,TN1M,TNK1M,WL,AC,PC
              REAL TNKS,TNM,TNO,TNS
              REAL TNK1I,TN1I,T1I,TNI,TNKI,TI,DTNK,DTN,D1T,DTN1
              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     16 READ 17,TNO,WL,TNS,TNKS,PHI1
    40        IF (TNO) 3000, 3000, 6
    42      6 READ  9, TNI,DTN,TNM,TNKI,DTNK,TNKM
    62      7 READ 11, TI,DT,TM
    74      5 READ 9,TN1I,DTN1,TN1M,TNK1I,DTNK1,TNK1M
   114      8 READ 11,T1I,D1T,T1M
            9 FORMAT (F9.0,5F10.0)
           11 FORMAT (F9.0, 2F10.0)
           17 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 FILM2= , F7.4, 2X,
             C 4H-  I, F7.4//18H FILM2 THICKNESS= , F7.2, 10H ANGSTROMS,
             C //8H PSIC = , F10.5, 10X, 7HDELC = , F10.5,
             C //8H AC    = ,F10.5,10X, 7HPC    = ,F10.5)
           25 FORMAT (1H0, 28HREFRACTIVE INDEX OF FILM1 = ,F7.4, 2X,
             C4H-  I, F7.4//19H FILM1 THICKNESS = , F7.2, 10H ANGSTROMS)
   126        PHI = 0.01745329252*PHI1
   130        CP = COS(PHI)
   132        SP = SIN(PHI)
   135        TN3 = CMPLX(TNS,-TNKS)
   140        LNK=TNK1I
   141     23 LN=TN1I
   143     22 L=T1I
   145     21 TN=TNI
   147     20 TNK=TNKI
   151     30 T = TI
   153    100 TN2 = CMPLX(TN,-TNK)
   156        TN1 = CMPLX(LN, -LNK)
   161        SC = (TNO*SP)/TN1
   172        CC = CSQRT(1. - SC*SC)
   203        CPHI3 = CSQRT(1.0 - TN1**2*SC**2/(TN3**2))
   236        CPHI2 = CSQRT(1.0 - TN1**2*SC**2/(TN2**2))
   271        R1S = (TN1*CC - TN2*CPHI2)/(TN1*CC + TN2*CPHI2)
```

```
DUALF
   330        R1P =-(TN1*CPHI2 - TN2*CC)/(TN1*CPHI2 + TN2*CC)
   366        R2S = (TN2*CPHI2 - TN3*CPHI3)/(TN2*CPHI2 + TN3*CPHI3)
   425        R2P =-(TN2*CPHI3 - TN3*CPHI2)/(TN2*CPHI3 + TN3*CPHI2)
   463        D = (0.0,1.0)*(4.0*3.1415927*T/WL)*TN2*CPHI2
   501        RS= (R1S + R2S*CEXP(-D))/(1.0 + R1S*R2S*CEXP(-D))
   540        RP = (R1P + R2P*CEXP(-D))/(1.0 + R1P*R2P*CEXP(-D))
   600        RHO = RP/RS
   607        S1 = SC
   612        T1 = SC/CC
   621        T2=(1. + RHO)/((1. - RHO)*T1)
   647        S2=T2/CSQRT(1. + T2*T2)
   670        LN3=(TN1*S1)/S2
   705        CPHI3 = CSQRT(1.0 - TNO**2*SP**2/(LN3**2))
   730        LN2=CMPLX(LN,-LNK)
   733        CPHI2 = CSQRT(1.0 - TNO**2*SP**2/(LN2**2))
   756        R1S = (TNO*CP - LN2*CPHI2)/(TNO*CP + LN2*CPHI2)
  1010        R1P =-(TNO*CPHI2 - LN2*CP)/(TNO*CPHI2 + LN2*CP)
  1041        R2S = (LN2*CPHI2 - LN3*CPHI3)/(LN2*CPHI2 + LN3*CPHI3)
  1100        R2P =-(LN2*CPHI3 - LN3*CPHI2)/(LN2*CPHI3 + LN3*CPHI2)
  1136        D = (0.0,1.0)*(4.0*3.1415927*L/WL)*LN2*CPHI2
  1154        RS= (R1S + R2S*CEXP(-D))/(1.0 + R1S*R2S*CEXP(-D))
  1213        RP = (R1P + R2P*CEXP(-D))/(1.0 + R1P*R2P*CEXP(-D))
  1252        RHO = RP/RS
  1262        PSIC = ATAN(CABS(RHO))/0.01745329252
  1266        DELC = ATAN2(AIMAG(RHO), REAL(RHO))/0.01745329252
  1276        AC = PSIC + 90.
  1277          PC = (90. - DELC)/2.
  1301        IF (DELC) 140,140,300
  1303    140 DELC = DELC + 360.00
  1305    300 PRINT 13, PHI1,TNC,WL,TNS,TNKS
  1323        PRINT 25,LN,LNK,L
  1335        PRINT 14, TN,TNK,T,PSIC,DELC,AC,PC
  1357    400 IF(TM -T) 600,600,500
  1362    500 T = T + DT
  1364        GO TO 100
  1365    600 IF(TNKM - TNK) 800,800,700
  1370    700 TNK = TNK + DTNK
  1372        GO TO 30
  1373    800 IF(TNM - TN)  910, 910,900
  1376    900 TN = TN + DTN
  1400        GO TO 20
  1401    910 IF (T1M - L) 930,930,920
  1404    920 L=L+D1T
  1406        GO TO 21
  1407    930 IF (TN1M - LN) 950,950,940
  1412    940 LN=LN+DTN1
  1414        GO TO 22
  1415    950 IF (TNK1M - LNK) 970,970,960
  1420    960 LNK=LNK+DTNK1
  1422        GO TO 23
  1423    970 GO TO 1
  1424   3000 CONTINUE
  1425        END
```

EXAMPLE OF OUTPUT

```
PHI = 75.00           N =  1.3500          WAVELENGTH =  5461  ANGSTROMS
 REFRACTIVE INDEX OF SUBSTRATE =   .9300  -  I 2.3900
 REFRACTIVE INDEX OF FILM1 =  1.4500  -  I-0.0000
 FILM1 THICKNESS =   -0.00 ANGSTRCMS
 REFRACTIVE INDEX OF FILM2=  2.7500  -  I  .250C
 FILM2 THICKNESS=   -0.00 ANGSTROMS
 PSIC =   37.62461          DELC =   58.93017
 AC   =  127.62461          PC   =   15.53492

PHI = 75.00           N =  1.3500          WAVELENGTH =  5461  ANGSTROMS
 REFRACTIVE INDEX OF SUBSTRATE =   .9300  -  I 2.3900
 REFRACTIVE INDEX OF FILM1 =  1.4500  -  I-0.0000
 FILM1 THICKNESS =   -0.00 ANGSTRCMS
 REFRACTIVE INDEX OF FILM2=  2.7500  -  I  .2500
 FILM2 THICKNESS=   50.00 ANGSTROMS
 PSIC =   38.47673          DELC =   52.17989
 AC   =  128.47673          PC   =   18.91005

PHI = 75.00           N =  1.3500          WAVELENGTH =  5461  ANGSTROMS
 REFRACTIVE INDEX OF SUBSTRATE =   .9300  -  I 2.3900
 REFRACTIVE INDEX OF FILM1 =  1.4500  -  I-0.0000
 FILM1 THICKNESS =   -0.00 ANGSTROMS
 REFRACTIVE INDEX OF FILM2=  2.75C0  -  I  .250C
 FILM2 THICKNESS=  100.00 ANGSTROMS
 PSIC =   39.72852          DELC =   47.08963
 AC   =  129.72852          PC   =   21.45519
```

II. FORTRAM IV COMPUTER PROGRAM "MULTF"

This program computes the ellipsometer data ψ and Δ for a system of a substrate covered with m films of monotonically varying refractive index, but of equal thickness.[1] It is based on the same principle as program "DUALF" (see Chapter I). As in program "DUALF" one starts out with the substrate S covered with Film "m " and assumes Film "m-1" as the incident medium (Fig. 2). The program computes the reflexion coefficient ρ_m of this first sub system (Substrate/Film "m"/Film "m-1"). This reflection coefficient ρ_m is converted into an effective refractive index n_{sm}, which serves as the substrate in the second step. In this second step Film "m -1" will serve as the covering film, while Film "m -2" is assumed to be the incident medium. The thickness of each film is assumed to be the same. This procedure is repeated m times until the prescribed number of Films m is reached.

A. Variables Used in the Program MULTF

NAme	Description
AC	Analyzer azimuth (zone A3)
DELC	Ellipsometric parameter Δ
DI	Decrement of imaginary part of refractive index of film-layers (between two successive layers)
DR	Decrement of real part of refractive index of film-layers
K	Number of film-layers of thickness T (referred to as m)
PC	Polarizer azimuth (zone A3)
PHI1	Angle of incidence ϕ
PSIC	Ellipsometric parameter ψ
T	Thickness of individual film-layer

Name	Description
TNI	Real part of refractive index of first layer
TNKI	Imaginary part of refractive index of first layer
TNKS	Imaginary part of refractive index of substrate
TNO	Refractive index of incident medium (real)
TNS	Real part of refractive index of substrate
WL	Wavelength

B. Input Format for Program MULTF

Card	1-9	10-19	20-29	30-39	40-49	50-59
1 2	Title and comments (up to 80 columns)					
3	TNO	WL	TNS	TNKS	PHI1	
4	TNI	TNKI	DR	DI	T	K (column 50-52)

These four cards constitute a set. Any number of sets may follow. Three blank cards must follow the last set of data. Note, that the number of films K is an integer variable of three digits (colmn 50-52).

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

```
      PROGRAM MULTF (INPUT,OUTPUT)
C     THIS PROGRAM CALCULATES THE ELLIPSOMETRIC PARAMETERS
C     DELC,PSIC OF A SUBSTRATE COVERED WITH MULTIPLE FILMS
C     OF EQUAL THICKNESS, BUT OF A STEPWISE CHANGE
C     OF THE COMPLEX REFRACTIVE INDEX
C     THE INCIDENT MEDIUM HAS THE REAL REFRACTIVE INDEX TNO
C     THE COMPUTATION STARTS FROM THE BOTTOM (SUBSTRATE)
C     AC AND PC ARE VALID FORE ZONE A3
      COMPLEX T2,S2,TN3,D
      COMPLEX TN2,      CPHI2, CPHI3, R1S, R1P, R2S, R2P,     RS, RP, RHO
      REAL PHI1,PHI,CP,SP,LNK,LN,L,TN,TNK,T,PSIC,DELC,DT,TM
      REAL DTNK1,TNKM,T1M,TN1M,TNK1M,WL,AC,PC
      REAL TNKS,TNM,TNO,TNS
      REAL TNK1I,TN1I,T1I,TNI,TNKI,TI,DTNK,DTN,D1T,DTN1
      DIMENSION TITLE (8), RANGE (8)
    1 READ 2, TITLE,RANGE
    2 FORMAT (8A10/8A10)
    3 PRINT 4, TITLE,RANGE
    4 FORMAT (1H1, 8A10//8A10)
   16 READ 17,TNO ,WL,TNS,TNKS,PHI1
      IF (TNO) 3000, 3000, 6
    6 READ 9, TNI,TNKI,DR,DI,T ,K
    9 FORMAT (F9.0,4F10.0,I3)
   17 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, 31HREFRACTIVE INDEX OF TOP FILM = , F7.4, 2X,
     C 4H-  I, F7.4//18H FILM  THICKNESS= , F7.2, 10H ANGSTROMS,
     C //23HNUMBER OF FILM-LAYER = I3,
     C //8H PSIC = , F10.5, 10X, 7HDELC = , F10.5,
     C //8H AC   = ,F10.5,10X, 7HPC   = ,F10.5)
      J = K + 1
      PHI = 0.01745329252*PHI1
      CP = COS(PHI)
      SP = SIN(PHI)
      TN3 = CMPLX(TNS,-TNKS)
   21 TN=TNI
   20 TNK=TNKI
      TN1 = TNO
      N = 0
      U = 0.
      R = 0.
  501 CONTINUE
  502 TN2 = CMPLX(TN,-TNK)
      SC = SP
      CC = CP
      CPHI3 = CSQRT(1.0 - TN1**2*SC**2/(TN3**2))
      CPHI2 = CSQRT(1.0 - TN1**2*SC**2/(TN2**2))
      R1S = (TN1*CC - TN2*CPHI2)/(TN1*CC + TN2*CPHI2)
      R1P =-(TN1*CPHI2 - TN2*CC)/(TN1*CPHI2 + TN2*CC)
      R2S = (TN2*CPHI2 - TN3*CPHI3)/(TN2*CPHI2 + TN3*CPHI3)
      R2P =-(TN2*CPHI3 - TN3*CPHI2)/(TN2*CPHI3 + TN3*CPHI2)
      D = (0.0,1.0)*(4.0*3.1415927*R/WL)*TN2*CPHI2
      RS= (R1S + R2S*CEXP(-D))/(1.0 + R1S*R2S*CEXP(-D))
```

```
      RP = (R1P + R2P*CEXP(-D))/(1.0 + R1P*R2P*CEXP(-D))
      RHO = RP/RS
      PSIC = ATAN(CABS(RHO))/0.01745329252
      DELC = ATAN2(AIMAG(RHO), REAL(RHO))/0.01745329252
      AC = PSIC + 90.
        PC = (90. - DELC)/2.
      IF (DELC) 140,140,300
  140 DELC = DELC + 360.00
  300 PRINT 13, PHI1,TNO,WL,TNS,TNKS
      R = U*T
      PRINT 14, TN ,TNK,R,N,PSIC,DELC,AC,PC
      S1 = SC
      T1 = SC/CC
      T2=(1. + RHO)/((1. - RHO)*T1)
      S2=T2/CSQRT(1. + T2*T2)
      TN3=(TN1*S1)/S2
      TN = TN - DR
      TNK = TNK - DI
      N = N + 1
      U = U + 1.
      IF (N - J) 501,3000,3000
 3000 CONTINUE
      END
```

EXAMPLE OF OUTPUT

```
 TEXT     *** 3 ***

 MULTFILM

PHI = 75.00      N = 1.3500     WAVELENGTH = 5461 ANGSTROMS
 REFRACTIVE INDEX OF SUBSTRATE =  .9800 - I 2.3900
 REFRACTIVE INDEX OF TOP FILM =  2.7650 - I  .2500
 FILM THICKNESS = 0.00 ANGSTROMS
 NUMBER OF FILM-LAYER = 0
 PSIC = 37.62461     DELC = 58.93017
 AC =  127.62461     PC   = 15.58492
PHI = 75.00      N = 1.3500     WAVELENGTH = 5461 ANGSTROMS
 REFRACTIVE INDEX OF SUBSTRATE =  .9800 - I 2.3900
 REFRACTIVE INDEX OF TOP FILM =  2.7500 - I  .2500
 FILM THICKNESS = 100.00 ANGSTROMS
 NUMBER OF FILM-LAYER = 1
 PSIC = 37.62461     DELC = 58.93017
 AC =  127.62461     PC   = 15.53492
PHI = 75.00      N = 1.3500     WAVELENGTH = 5461 ANGSTROMS
 REFRACTIVE INDEX OF SUBSTRATE =  .9800 - I 2.3900
 REFRACTIVE INDEX OF TOP FILM =  2.7350 - I  .2500
 FILM THICKNESS = 200.00 ANGSTROMS
 NUMBER OF FILM-LAYER = 2
 PSIC = 39.72939     DELC = 46.01971
 AC =  129.72939     PC   = 21.99015
```

ACKNOWLEDGEMENTS

This work was conducted under the auspices of the U. S. Atomic Energy Commission. I wish to thank the Deutsche Forschungsgemeinschaft for its financial support.

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2. H. J. Mathieu, Computer Programs for Ellipsometry, LBL-1470, University of California, Berkeley, 1973.
3. R. H. Muller in Advances in Electrochemistry and Electrochemical Engineering, Vol. 9, R. H. Muller, ed. (Wiley-Interscience, N. Y., 1973), p. 167f.

FIGURE CAPTIONS

Fig. 1. (a) Model for a two-film coverage of the substrate.

(b) Step 1. Film 1 is assumed to be the incident medium.

(c) Step 2, using the new refractive index n_s' (Step 1) as effective refractive index of an apparent substrate S', Film 1 is assumed to cover the substrate S'.

Fig. 2. Inhomogeneous film represented by m layers of equal thickness with increments in optical constants Δn and Δk between successive layers.

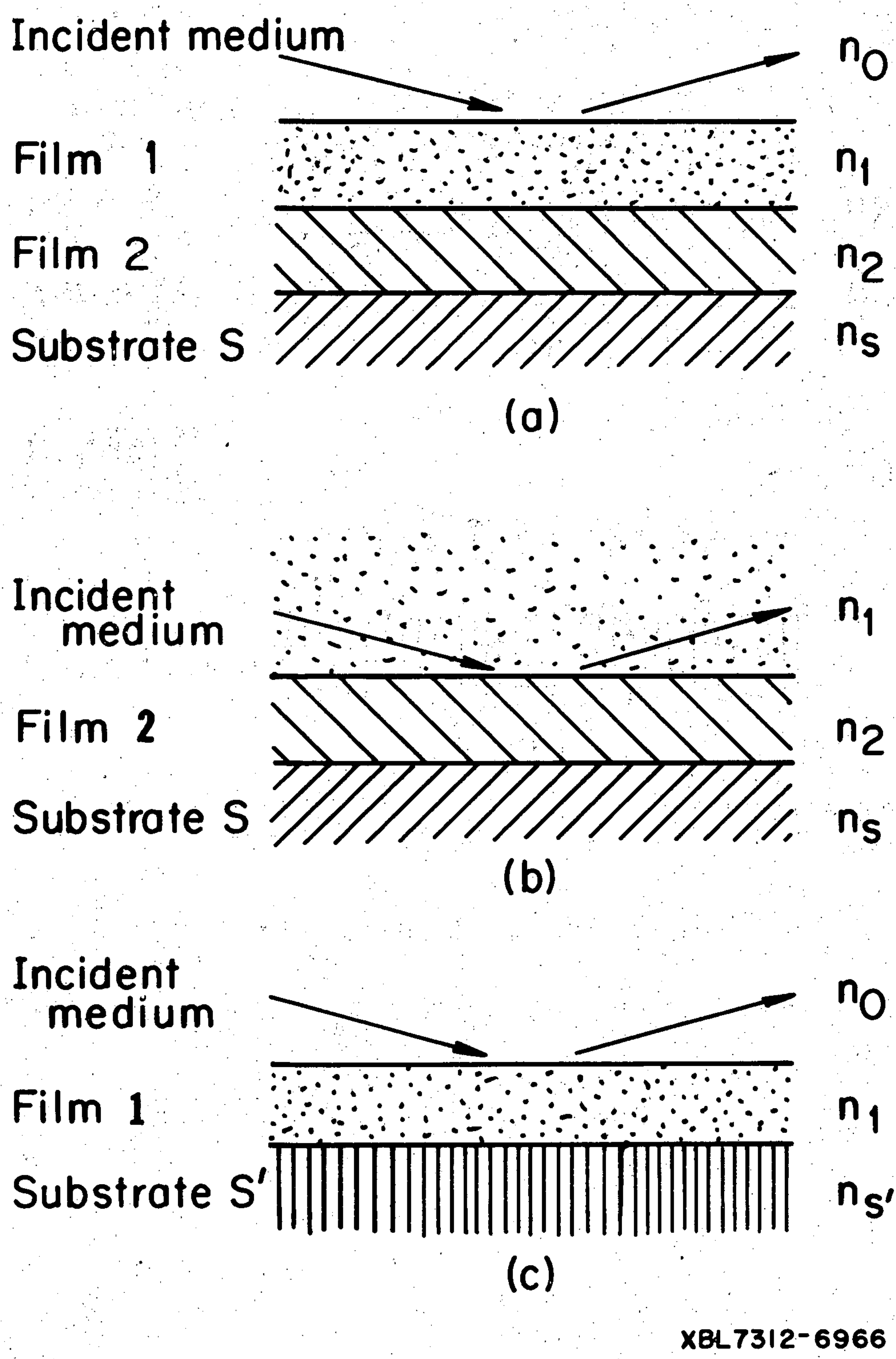
Incident medium
n_0
Film 1
n_1
Film 2
n_2
Substrate S
n_s
(a)
Incident medium
n_1
Film 2
n_2
Substrate S
n_s
(b)
Incident medium
n_0
Film 1
n_1
Substrate S′
$n_{s'}$
(c)
XBL7312-6966

Fig. 1

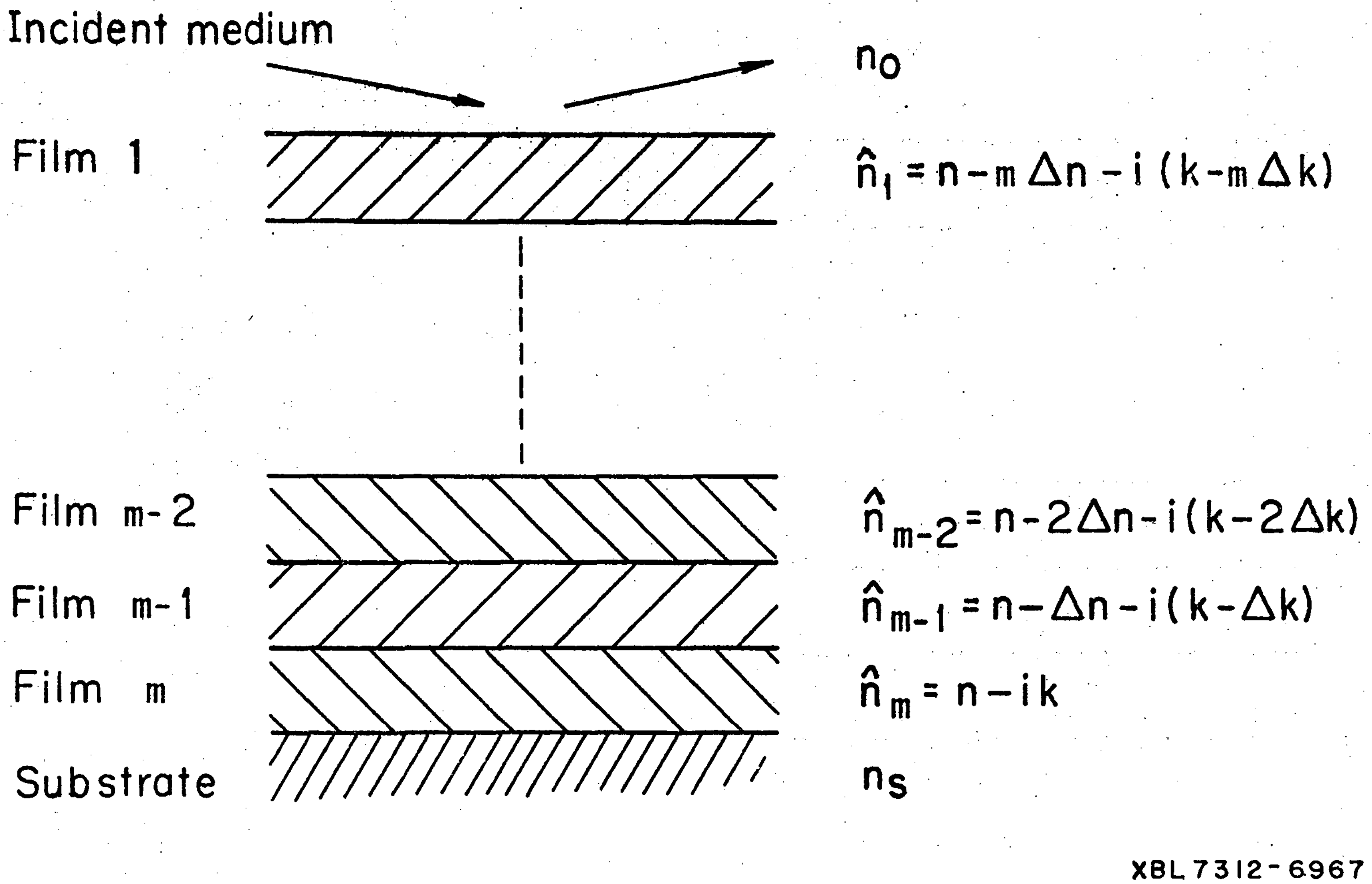
Incident medium
n_0
Film 1
$\hat{n}_1 = n - m\Delta n - i(k - m\Delta k)$
Film m-2
$\hat{n}_{m-2} = n - 2\Delta n - i(k - 2\Delta k)$
Film m-1
$\hat{n}_{m-1} = n - \Delta n - i(k - \Delta k)$
Film m
$\hat{n}_m = n - ik$
Substrate
n_s
XBL 7312-6967

Fig. 2

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