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REFLECTION OF POLARIZED LIGHT FROM ABSORBING MEDIA

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August 1966

ABSTRACT

Reflection of polarized light from absorbing media, such as a bare metal surface in contact with a dielectric, results in characteristic changes in the polarization state from which the optical constants of the reflecting interface can be determined. Starting from Maxwell's equations of electromagnetic theory, the basic relationships of metallic reflection and exact formulas for relating the optical constants with amplitude and phase changes upon reflection are derived and illustrated by extensive numerical data.

magnetic dipole moment per unit volume),  $\vec{J}_{\text{free}}$  is the free current density,  $\vec{H}$  is the magnetic field intensity,  $\frac{\partial \vec{D}}{\partial t}$  is the displacement current density,  $\rho_{\text{free}}$  is the free charge density,  $\vec{D}$  is the displacement vector, and  $c$  is the speed of light in vacuum.

At the outset, the following assumptions\* will be made:

1.  $\vec{E}$ ,  $\vec{D}$ ,  $\vec{P}$ ,  $\vec{B}$ ,  $\vec{H}$ ,  $\vec{M}$  and  $\vec{J}_{\text{free}}$  oscillate sinusoidally\*\* at each point with frequency  $\omega$ . That is,

$$\begin{aligned} \vec{E} &= \vec{E}_s e^{-i\omega t} & \vec{P} &= \vec{P}_s e^{-i\omega t} \\ \vec{B} &= \vec{B}_s e^{-i\omega t} & \vec{M} &= \vec{M}_s e^{-i\omega t} \end{aligned} \quad (7a-g)$$

$$\vec{J}_{\text{free}} = \vec{J}_s e^{-i\omega t} \quad \vec{D} = \vec{D}_s e^{-i\omega t} \quad \vec{H} = \vec{H}_s e^{-i\omega t}$$

where the subscript  $s$  refers to the time independent quantity in each case.

2. The media to be considered are all linear and isotropic, that is,

$$\vec{P}_s = \chi_e \vec{E}_s, \quad \vec{M}_s = \chi_m \vec{H}_s, \quad \vec{J}_s = \sigma \vec{E}_s \quad (8a-c)$$

and the magnetic and electric susceptibilities  $\chi_m$  and  $\chi_e$  as well as the conductivity  $\sigma$  are constant throughout each medium.

3. The equation of continuity holds, i.e.,

$$\frac{\partial \rho_{\text{free}}}{\partial t} = -\text{div } \vec{J}_{\text{free}} = -e^{-i\omega t} \text{div } \vec{J}_s$$

\* This treatment is given in Ref. 1, pp. 369-372.

\*\* The choice of  $e^{-i\omega t}$  instead of  $e^{+i\omega t}$  to represent the time dependence is arbitrary, but is in keeping with current practice.

When this equation is integrated with respect to time, there results,

$$\rho_{\text{free}} = \rho_s e^{-i\omega t}$$

where

$$\rho_s = -\frac{i}{\omega} \operatorname{div} \vec{J}_s = -\frac{i}{\omega} \operatorname{div} \sigma \vec{E}_s \quad (9)$$

Having made these assumptions, it is now possible to eliminate the time dependence from Eqs. (1) through (4). Substituting Eqs. (8a-b) into Eqs. (7a-d), then into Eqs. (5) and (6) and dividing out the common factor  $e^{-i\omega t}$  leaves

$$\vec{D}_s = (1 + 4\pi\chi_e) \vec{E}_s \quad (5a)$$

$$\vec{B}_s = (1 + 4\pi\chi_m) \vec{H}_s \quad (6a)$$

so that

$$\vec{D}_s = \epsilon \vec{E}_s \quad (5b)$$

$$\vec{B}_s = \mu \vec{H}_s \quad (6b)$$

Due to the assumption 2 above,  $\epsilon$  and  $\mu$  will be considered as constants for each medium.

Substituting Eqs. (5b) and (9) into Eq. (1) gives

$$\operatorname{div} \left( \epsilon + \frac{4\pi\sigma}{\omega} i \right) \vec{E}_s = 0 \quad (1a)$$

Since

$$\frac{\partial \vec{B}}{\partial t} = -i\omega \vec{B}_s e^{-i\omega t} = -i\omega \mu \vec{H}_s e^{-i\omega t} \quad (10)$$

Equation (2) can be written, cancelling the common factor  $e^{-i\omega t}$ , as

$$\operatorname{curl} \vec{E}_s = \frac{i\omega\mu}{c} \vec{H}_s \quad (2a)$$



with Eq. (6b), Eq. (3) becomes, dividing out the factor  $e^{-i\omega t}$ ,

$$\text{div } \mu \vec{H}_s = 0. \quad (3a)$$

Finally, using Eqs. (5b), (7e) and (8c) and cancelling the factor  $e^{-i\omega t}$ , Eq. (4) can be written

$$\text{curl } \vec{H}_s = -i \frac{\omega}{c} \left( \epsilon + i \frac{4\pi\sigma}{\omega} \right) \vec{E}_s \quad (4a)$$

Taking the curl of Eq. (2a) and substituting  $\text{curl } \vec{H}_s$  from Eq. (4a) one has

$$\text{curl curl } \vec{E}_s = \frac{\omega^2 \mu}{c^2} \left( \epsilon + i \frac{4\pi\sigma}{\omega} \right) \vec{E}_s \quad (11)$$

Applying the vector identity\*

$$\text{curl curl } \vec{E}_s = \text{grad div } \vec{E}_s - \nabla^2 \vec{E}_s$$

where, if  $x$ ,  $y$ , and  $z$  are cartesian coordinates

$$\nabla^2 \vec{E}_s = \frac{\partial^2 \vec{E}_s}{\partial x^2} + \frac{\partial^2 \vec{E}_s}{\partial y^2} + \frac{\partial^2 \vec{E}_s}{\partial z^2}$$

and noting that by Eq. (1a)

$$\text{div } \vec{E}_s = 0$$

since  $\epsilon$  and  $\sigma$  are independent of position, there results

$$\nabla^2 \vec{E}_s + \frac{\omega^2}{c^2} \mu \left( \epsilon + i \frac{4\pi\sigma}{\omega} \right) \vec{E}_s = 0. \quad (12)$$

Equation (12) is the wave equation.

\* See Reference 1, p. 27.

### C. Solution of Wave Equation

Equation (12) can be simplified by making the definition

$$n_c^2 \equiv \mu \left( \epsilon + i \frac{4\pi\sigma}{\omega} \right) \quad (13)$$

so that

$$\nabla^2 \vec{E}_s + \frac{\omega^2}{c^2} n_c^2 \vec{E}_s = 0 \quad (12a)$$

The complex quantity  $n_c$  is called the complex index of refraction further defined by

$$n_c \equiv n (1 + i\kappa)^* \quad (14)$$

\* In the literature one often finds these other forms for the complex index of refraction:

$$n_c = n + i\kappa \quad (14a)$$

$$n_c = n - i\kappa \quad (14b)$$

$$n_c = n(1 - i\kappa) \quad (14c)$$

Definitions (14b) and (14c) are rejected here because, together with choosing the sinusoidal time variation as  $e^{-i\omega t}$ , they would lead to the definition of an intrinsically negative absorption coefficient (see Eqs. (27b), (22a) and (17) below). If, on the other hand, one uses  $e^{+i\omega t}$  to describe the time dependence of the fields, then one should represent the complex index of refraction by either Eq. (14b) or (14c). The choice made here, namely Eq. (14), is made to facilitate comparison of later equations with those given in the literature (see also Appendix I).

It will be shown in this section that the real quantities  $n$  and  $\kappa$  are related to the ratio  $n'$  of the phase velocity in the medium under consideration to that in vacuum and to the absorption coefficient  $\alpha$  which is a measure of the energy absorbed when an electromagnetic wave passes through the medium.

To solve the wave equation one assumes a solution of the form

$$\vec{E}_s(x,y,z) = \vec{E}_0 e^{i(\mu_1 x + \mu_2 y + \mu_3 z)} \quad (15)$$

where  $x, y, z$  are measured from an arbitrary reference 0. In Eq. (15)  $\mu_1, \mu_2,$  and  $\mu_3$  are constants, in general complex, and  $\vec{E}_0$  is a constant vector, also complex in general. Substitution of Eq. (15) into Eq. (12a) leads to the relation

$$\frac{\omega^2}{c^2} n_c^2 = \mu_1^2 + \mu_2^2 + \mu_3^2 \quad (16)$$

Since  $n_c$  is complex,  $\mu_1, \mu_2,$  and  $\mu_3$  cannot all be real.

### 1. Transparent Media

When an electromagnetic wave propagates through a transparent medium ( $\sigma = 0$ ) the solution to the wave equation is of the form

$$\vec{E}_s(x,y,z) = \vec{E}_0 e^{i\vec{k} \cdot \vec{r}}$$

where  $\vec{r}$  is a vector from an arbitrary reference point to the point of interest  $(x,y,z)$  and  $\vec{k}$  is a real quantity giving the direction of propagation. The magnitude of  $\vec{k}$  is

$$k = \frac{\omega}{v}$$

where  $v$  is the phase velocity of the wave. Planes of equal phase and planes of equal amplitude are normal to  $\vec{k}$ .

## 2. Absorbing Media

As discussed by Ditchburn\* and Stone\*\* when the medium is absorbing, planes of equal phase are normal to the direction of propagation  $\vec{k}$ , (Fig. 1) while planes of equal amplitude are parallel to the plane surface of the medium (normal to another direction  $\vec{a}$ ). For such a medium, the solution of Eq. (12a) may be written

$$\vec{E}_s = \vec{E}_0 e^{-\alpha z} e^{i\vec{k} \cdot \vec{r}} \quad (17)$$

Equation (17) represents a plane wave, moving in the direction of  $\vec{k}$ , that is reduced in amplitude as it passes through the medium. After travelling to a depth  $z = \frac{1}{2\alpha}$  (known as the penetration depth), the intensity is diminished by a factor of  $1/e$ .

The constant  $\alpha$  is called the absorption coefficient and is taken positive by definition. With the inward normal to the surface of the reflecting medium oriented along the positive  $z$  axis, as shown in Fig. 1, the plane of incidence (the plane defined by  $z$  and  $\vec{k}$ ) is the  $xz$  plane. Let  $\vec{k}$  make an angle  $\phi_r$  with the  $z$  axis.

From Fig. 1,

$$\vec{k} = k(\hat{x} \sin \phi_r + \hat{z} \cos \phi_r) \quad (18)$$

$$\vec{r} = x\hat{x} + y\hat{y} + z\hat{z} \quad (19)$$

$$k = |\vec{k}|$$

In all equations, the symbol " $\hat{\phantom{x}}$ " over a letter denotes a unit vector along the axis denoted by the letter. By Eq. (18) and (19),

$$\vec{k} \cdot \vec{r} = k(x \sin \phi_r + z \cos \phi_r)$$

By definition,\* the ratio of the vacuum phase velocity  $c$  to the phase

\* Ref. 11, p. 590.

\*\* Ref. 1, p. 392.

velocity  $v$  in the medium is the real index of refraction  $n'$ .

$$\frac{c}{v} \equiv n' \geq 0 \quad (20)$$

Thus

$$k \equiv \frac{\omega}{v} = \frac{\omega}{c/n'} = \frac{\omega}{c} n' = k_0 n' \quad (20a)$$

Here the subscript 0 denotes the value of the subscripted quantity in vacuum.

Equation (17) can now be written

$$\vec{E}_s = \vec{E}_0 e^{-\alpha z} e^{i \frac{\omega n'}{c} (x \sin \phi_r + z \cos \phi_r)}$$

or

$$\vec{E}_s = \vec{E}_0 e^{i \left[ \frac{\omega n'}{c} (x \sin \phi_r + z \cos \phi_r) + i \alpha z \right]} \quad (21)$$

It is useful to define  $\kappa'$  so that

$$\kappa' \equiv \frac{\alpha}{k} = \frac{\alpha c}{\omega n'} \geq 0 \quad (22)$$

and to define  $n'_c$  by

$$n'_c \equiv n' (1 + i \kappa')$$

Equations (27a) and (27b) which will presently be derived relate  $n'$  and  $\kappa'$  to  $n$  and  $\kappa$ . Thus  $n'_c$  can also be considered as a complex index of refraction although not equivalent to  $n_c$ .

The solution of Eq. (22) for the absorption coefficient  $\alpha$  results in

$$\alpha = \frac{\omega n' \kappa'}{c} = \frac{2\pi n' \kappa'}{\lambda_0} \geq 0^* \quad (22a)$$

where  $\lambda_0$  is the vacuum wavelength.

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\* The absorption coefficient usually found in the literature is twice that given by Eq. (22a), e.g. Ref. [5] p. 614. The reason for the difference is that the absorption coefficient is usually regarded as the inverse of the distance travelled by the wave when the intensity decreases by 1/e. Since the intensity is proportional to the squared modulus of the electric field,

$$I \propto |E|^2$$

one has, from Eq. (17),  $I \propto e^{-2\alpha z}$ . Hence, the intensity diminishes by an amount 1/e after penetrating to a depth  $z = 1/2\alpha$ .

With these new definitions, Eq. (21) becomes

$$\vec{E}_s = \vec{E}_0 e^{i\left[\frac{\omega n'}{c}(x \sin \phi_r + z \cos \phi_r) + \frac{i\omega n' \kappa' z}{c}\right]} \quad (21a)$$

$$\vec{E}_s = \vec{E}_0 e^{i\frac{\omega n'}{c}[x \sin \phi_r + z(\cos \phi_r + i\kappa')]} \quad (21b)$$

An alternative and somewhat simpler way of handling the solution to Eq. (12a) and one that will be used in later sections is to introduce the complex propagation vector  $\vec{k}_c$ ,

$$\vec{k}_c = \vec{k} + i\vec{a} \quad (23)$$

where  $\vec{a}$  is called the attenuation vector. As mentioned above, planes of equal amplitude are normal to  $\vec{a}$ .

$$\vec{a} = |\vec{a}|\hat{z} = a\hat{z}$$

By analogy with the plane wave solution one writes

$$\vec{E}_s = \vec{E}_0 e^{i\vec{k}_c \cdot \vec{r}} \quad (24)$$

When Eqs. (23), (18), and (19) are substituted into Eq. (24), there results

$$\vec{E} = \vec{E}_s e^{-i\omega t} = E_0 e^{-i[\omega t - k(x \sin \phi_r + z \cos \phi_r) - iaz]} \quad (25)$$

or, since  $k = n' k_0 = \frac{n'\omega}{c}$

$$\vec{E}_s = \vec{E}_0 e^{i\left[\frac{\omega n'}{c}(x \sin \phi_r + z \cos \phi_r) + iaz\right]} \quad (25a)$$

Comparison of Eqs. (25a) and (21a) shows

$$a = \frac{\omega n' \kappa'}{c} = \alpha \quad (26)$$

It is important to keep in mind that  $n \neq n'$  and  $\kappa \neq \kappa'$ . The following discussion will make this point clear.

Equation (21b) is in the form of Eq. (15) with

$$\mu_1 = \frac{\omega n'}{c} \sin \phi_r$$

$$\mu_2 = 0$$

$$\mu_3 = \frac{\omega n'}{c} (\cos \phi_r + i\kappa')$$

Substituting into Eq. (16),

$$\frac{\omega^2 n^2}{c^2} = \frac{\omega^2}{c^2} n'^2 \sin^2 \phi_r + \frac{\omega^2 n'^2}{c^2} (\cos \phi_r + i\kappa')^2$$

$$n^2(1-\kappa^2) + 2in^2\kappa = n'^2 \sin^2 \phi_r + n'^2(\cos^2 \phi_r - \kappa'^2) + 2i\kappa'n'^2 \cos \phi_r$$

Equating real parts,

$$n^2(1 - \kappa^2) = n'^2(1 - \kappa'^2) \quad (27a)$$

Equating imaginary parts,

$$n^2 \kappa = n'^2 \kappa' \cos \phi_r \quad (27b)$$

Equations (27a) and (27b) show that

$$n \neq n'$$

$$\kappa \neq \kappa'$$

unless  $\phi_r = 0$ , (i.e., unless incidence is normal) or  $\kappa = \kappa' = 0$  (non-absorbing media. Table 1 shows how  $n'$  and  $\kappa'$  differ from  $n$  and  $\kappa$  for the case of chromium ( $n = 2.96$ ,  $\kappa = 1.13$ ). Note that if one assumes  $n$  and  $\kappa$  to be independent of angle of incidence, then a slight dependence on incident angle is found for  $n'$  and  $\kappa'$ . Conversely, if one assumes  $n'$  and  $\kappa'$  are independent of incident angle, then a slight variation of  $n$  and  $\kappa$  with angle of incidence is found (see table 2). Included in Table 1 are the conductivity  $\sigma$ , the dielectric constant  $\epsilon$  and the



Table I

## OPTICAL CONSTANTS OF CHROMIUM

If the optical constants  $n$  and  $\kappa$  are assumed not to depend on angle of incidence  $\phi$ , the auxiliary constants  $n'$  and  $\kappa'$  do.

$\phi$ (deg)	$n$	$n'$	$\kappa$	$\kappa'$	$\sigma$ (gaussian)	$\epsilon$	Pen. Depth (cm)
45	2.960	3.007	1.130	1.126	$5.435 \times 10^5$	-2.429	$1.283 \times 10^{-6}$
55	2.960	3.024	1.130	1.125	5.435	-2.528	1.278
65	2.960	3.038	1.130	1.124	5.434	-2.427	1.273
75	2.960	3.049	1.130	1.123	5.434	-2.427	1.269
85	2.959	3.054	1.130	1.123	5.432	-2.427	1.268

$$\lambda = 5.461 \times 10^{-5} \text{ cm}$$

$\sigma$  = electrical conductivity

$\epsilon$  = dielectric constant

Table II

## OPTICAL CONSTANTS OF CHROMIUM

If the auxiliary optical constants  $n'$  and  $\kappa'$  are assumed not to depend on angle of incidence  $\phi$ , then the optical constants  $n$  and  $\kappa$  do.

(deg)	$n'$	$\kappa'$	$n$	$\kappa$
5	3.000	1.130	2.999	1.130
25	3.000	1.130	2.983	1.131
45	3.000	1.130	2.952	1.134
55	3.000	1.130	2.935	1.135
65	3.000	1.130	2.920	1.137
75	3.000	1.130	2.909	1.138
85	3.000	1.130	2.903	1.138

penetration depth  $\frac{1}{2\alpha}$  (in cm.). The conductivity and dielectric constant are found by squaring Eq. (14) and substituting for  $n_c^2$  in Eq. (13). Thus

$$n_c^2 = n^2(1 - \kappa^2) + i2n^2\kappa = \mu(\epsilon + \frac{4\pi\sigma}{\omega} i)$$

from which it follows, for  $\mu = 1$ , that

$$\epsilon = n^2(1 - \kappa^2)$$

$$\sigma = \frac{n^2\kappa\omega}{2\pi}$$

According to Ditchburn,\* when light is incident from a medium of real refractive index  $n'_0$  in which the phase velocity is  $v_0 = c/n'_0$ , then the angles of incidence  $\phi$  and refraction  $\phi_r$  (both real) are related by

$$\begin{aligned} \frac{\sin \phi}{\sin \phi_r} &= \frac{v_0}{v} \\ &= \frac{c/n'_0}{c/n'} = \frac{n'}{n'_0} \end{aligned}$$

or

$$n_0 \sin \phi = n' \sin \phi_r$$

This equation is formally the same as Snell's Law for a transparent medium. Thus, if one requires that  $n'$  and  $\kappa'$  be independent of incident angle ( $n$  and  $\kappa$  will then be dependent on incident angle), Snell's Law can be said to hold for absorbing media as well as for transparent media. Since  $n' \neq n$ , Snell's Law holds only for  $n'$  and not for  $n$ , i.e.,

$$n_0 \sin \phi \neq n \sin \phi_r$$

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\*Ref. 11, pp. 54, 590.

where  $n$  is the real part of

$$n_c = n(1 + i\kappa). \quad (14)$$

In summary, the spatial description of a plane electromagnetic wave travelling in an absorbing medium characterized by a real refractive index  $n' = \frac{c}{v}$  (where  $v$  is the phase velocity), and by a real absorption coefficient  $\alpha$ ,

$$\alpha = \frac{\omega n' \kappa'}{c}, \quad \kappa' = \frac{\alpha c}{\omega n'}$$

and travelling in the direction

$$\vec{k} = \frac{\omega}{v} (\hat{x} \sin \phi_r + \hat{z} \cos \phi_r)$$

is given by

$$\vec{E}_s = \vec{E}_0 e^{i \frac{\omega n'}{c} [x \sin \phi_r + z (\cos \phi_r + i\kappa')]}$$

When the time dependence is taken into consideration, the electric field is given by

$$\vec{E} = \vec{E}_s e^{-i\omega t} = \vec{E}_0 e^{-i \frac{2\pi}{\lambda_0} [ct - n'(x \sin \phi_r + z (\cos \phi_r + i\kappa'))]} \quad (21c)$$

where  $\frac{2\pi}{\lambda_0} = \frac{\omega}{c}$ ,  $\lambda_0 =$  vacuum wave length.

#### D. Reflection Coefficients for Absorbing Media

##### 1. Evaluation of Boundary Conditions

Consider a plane wave that is incident from a non-absorbing medium of real refractive index  $n_0 = n'_0$  onto the plane surface of an absorbing medium of complex index of refraction  $n_c = n(1 + i\kappa)$  or  $n'_c = n'(1 + i\kappa')$  related by Eqs. (27a) and (27b). Figure 2 shows the parallel and normal components of the incident, refracted and reflected waves  $\vec{E}$ ,  $\vec{E}'$ , and  $\vec{E}''$ .

The plane of incidence is the xz plane while the plane  $z = 0$  is the boundary between the two media. In the figure the subscript s refers to polarization normal to the plane of incidence, and the subscript p refers to polarization parallel to the plane of incidence.

Inspection of Fig. 2 shows that the electric fields of the incident and reflected waves can be written in the form of Eq. (21c) with  $\kappa = 0$  as

$$\vec{E} = (E_p \cos \phi \hat{x} + E_s \hat{y} - E_p \sin \phi \hat{z}) e^{\frac{-2\pi i}{\lambda_0} [ct - n_0(x \sin \phi + z \cos \phi)]} \quad (28)$$

$$\vec{E}'' = (E_p'' \cos \phi \hat{x} + E_s'' \hat{y} + E_p'' \sin \phi \hat{z}) e^{\frac{-2\pi i}{\lambda_0} [ct - n_0(x \sin \phi - z \cos \phi)]} \quad (29)$$

The quantities within the parentheses that precede the exponential factors of Eqs. (28) and (29) are the  $\vec{E}_0$ 's of Eq. (21c). They are found by resolving the electric field vector into components  $\vec{E}_p$  parallel to the plane of incidence and  $\vec{E}_s$  normal to the plane of incidence and then resolving these along the three coordinate axes.

For the refracted wave it can be assumed that  $\vec{E}'_0$  is of the form

$$\vec{E}'_0 = \epsilon'_1 E'_p \hat{x} + E'_s \hat{y} + \epsilon'_3 E'_p \hat{z} \quad (30)$$

where  $\epsilon_1$  and  $\epsilon_3$  may be complex. An  $\epsilon'_2$  could be used here with  $E'_s$ , but it would serve no purpose, and is hence assumed to be part of  $E'_s$ .

In order to evaluate the epsilons, Maxwell's Equations (1a), (2a), (3a), and (4a) will be rewritten. Using the identities\*

$$\text{curl} \cdot [\vec{C} e^{i\vec{k}_c \cdot \vec{r}}] = i\vec{k}_c \times \vec{C} e^{i\vec{k}_c \cdot \vec{r}}$$

\* See [1] problem 4-10 and page 372.

$$\text{div } \vec{C} e^{i\vec{k}_c \cdot \vec{r}} = i\vec{k}_c \cdot \vec{C} e^{i\vec{k}_c \cdot \vec{r}}$$

and assuming  $\vec{H}_s$  of the form

$$\vec{H}_s = \vec{H}_0 e^{i\vec{k}'_c \cdot \vec{r}}$$

where  $\vec{k}'_c$  is the complex wave vector for the second medium, Maxwell's equations become (setting  $\mu = 1$ )

$$\vec{k}_c \cdot \vec{E}_0 = 0 \tag{1b}$$

$$\frac{c}{\omega} \vec{k}_c \times \vec{E}_0 = \vec{H}_0 \tag{2b}$$

$$\vec{k}_c \cdot \vec{H}_0 = 0 \tag{3b}$$

$$-\frac{c}{\omega} \vec{k}_c \times \vec{H}_0 = n_c^2 \vec{E}_0 \tag{4b}$$

By Eqs. (23), (18), (19), and (26),

$$\vec{k}'_c = \frac{\omega n'}{c} [\hat{x} \sin \phi_r + \hat{z} (\cos \phi_r + ik')] \tag{31}$$

Using Eqs. (30), (31), Eq. (1b) becomes

$$[\hat{x} \sin \phi_r + \hat{z} (\cos \phi_r + ik')] \cdot [\epsilon_1 E'_p \hat{x} + E'_s \hat{y} + \epsilon_3 E'_p \hat{z}] = 0$$

$$0 = \epsilon_1 E'_p \sin \phi_r + \epsilon_3 E'_p (\cos \phi_r + ik')$$

$$\epsilon_1 \sin \phi_r = -\epsilon_3 (\cos \phi_r + ik')$$

One solution to this equation is

$$\epsilon_1 = \cos \phi_r + ik'$$

$$\epsilon_3 = -\sin \phi_r$$

The justification for choosing this solution will be the satisfaction of Maxwell's Equations (Eqs. (1b)-(4b)) by the resulting  $\vec{E}'_0$  and  $\vec{H}'_0$ .\*

Thus,

$$\vec{E}'_0 = E'_p (\cos \phi_r + i\kappa') \hat{x} + E'_s \hat{y} - E'_p \sin \phi_r \hat{z} \quad (32)$$

Using Eqs. (31), (32), and (2b), one obtains

$$\begin{aligned} \vec{H}'_0 &= n' [\hat{x} \sin \phi_r + \hat{z} (\cos \phi_r + i\kappa')] \times [E'_p (\cos \phi_r + i\kappa') \hat{x} + E'_s \hat{y} - E'_p \sin \phi_r \hat{z}] \\ &= n' [E'_s \sin \phi_r \hat{z} + E'_p \sin^2 \phi_r \hat{y} + E'_p (\cos \phi_r + i\kappa')^2 \hat{y} - E'_s (\cos \phi_r + i\kappa') \hat{x}] \\ \vec{H}'_0 &= n' [-E'_s (\cos \phi_r + i\kappa') \hat{x} + E'_p (1 - \kappa'^2 + 2i\kappa' \cos \phi_r) \hat{y} + E'_s \sin \phi_r \hat{z}] \quad (33) \end{aligned}$$

It can be shown by forming the product  $\vec{k}'_c \cdot \vec{H}'_0$  that Maxwell's equation (3b) is satisfied by Eq. (33), i.e.,

$$\vec{k}'_c \cdot \vec{H}'_0 = 0$$

In order to further show that  $\vec{H}'_0$  and  $\vec{E}'_0$  are correct as given by Eqs. (32) and (33), evaluation of the fourth Maxwell equation (4b) is carried out.

From Eqs. (31) and (33),

$$\begin{aligned} \frac{c}{\omega} \vec{k}'_c \times \vec{H}'_0 &= n'^2 [\hat{x} \sin \phi_r + \hat{z} (\cos \phi_r + i\kappa')] \times [-E'_s (\cos \phi_r + i\kappa') \hat{x} \\ &\quad + E'_p (1 - \kappa'^2 + i2\kappa' \cos \phi_r) \hat{y} + E'_s \sin \phi_r \hat{z}] \\ &= n'^2 [E'_p \sin \phi_r (1 - \kappa'^2 + i2\kappa' \cos \phi_r) \hat{z} - E'_s \sin^2 \phi_r \hat{y} - E'_s (\cos \phi_r + i\kappa')^2 \hat{y}] \end{aligned}$$

---

\* A vector field is uniquely specified if its curl and divergence are given. Maxwell's equations give the curl and divergence of  $\vec{E}$  and  $\vec{H}$ . Thus, if a particular  $\vec{E}$  and  $\vec{H}$  satisfy Maxwell's equations, they are the only solutions.

$$\begin{aligned}
 & - E'_p (\cos \phi_r + i\kappa')(1-\kappa'^2 + i2\kappa' \cos \phi_r) \hat{x} \\
 = & -n'^2 \left[ E'_p (\cos \phi_r + i\kappa') \hat{x} + E_s \hat{y} - E'_p \sin \phi_r \hat{z} \right] \cdot \left[ 1-\kappa'^2 + 2i\kappa' \cos \phi_r \right] \\
 = & -\vec{E}'_0 \left[ n'^2(1-\kappa'^2) + 2in'^2\kappa' \cos \phi_r \right]
 \end{aligned}$$

Substituting from Eqs. (27a) and (27b),

$$\begin{aligned}
 \frac{c}{\omega} \vec{k}_c \times \vec{H}_0 = \\
 -\vec{E}'_0 \left[ n'^2(1-\kappa'^2) + 2in'^2\kappa' \cos \phi_r \right] = -\vec{E}'_0 \left| n^2(1-\kappa^2) + 2in^2\kappa \right| = -n_c^2 \vec{E}'_0
 \end{aligned}$$

Thus  $\vec{E}'_0$  and  $\vec{H}'_0$  given by Eqs. (32) and (33) satisfy Maxwell's Equations.

All three electric fields  $\vec{E}$ ,  $\vec{E}'$ , and  $\vec{E}''$  may be written in the form of Eq. (21c). In Eq. (35) below, Snell's law

$$n_0 \sin \phi = n' \sin \phi_r \quad (34)$$

has been used in the exponent so that the coefficient of  $x$  is the same for all three fields

$$\vec{E} = (E_p \cos \phi \hat{x} + E_s \hat{y} - E_p \sin \phi \hat{z}) e^{-\frac{2\pi i}{\lambda_0} [ct - n_0 (x \sin \phi + z \cos \phi)]} \quad (28)$$

$$\vec{E}'' = (E''_p \cos \phi \hat{x} + E''_s \hat{y} + E'' \sin \phi \hat{z}) e^{-\frac{2\pi i}{\lambda_0} [ct - n_0 (x \sin \phi - z \cos \phi)]} \quad (29)$$

$$\vec{E}' = [E'_p (\cos \phi_r + i\kappa') \hat{x} + E'_s \hat{y} - E'_p \sin \phi_r \hat{z}] e^{-\frac{2\pi i}{\lambda_0} [ct - n_0 x \sin \phi + n'z(\cos \phi_r + i\kappa')]} \quad (35)$$

The magnetic fields  $\vec{H}$  and  $\vec{H}''$  corresponding to  $\vec{E}$  and  $\vec{E}''$  can be found by applying Maxwell's Equation (2b) to Eqs. (28) and (29) remembering that in the incident medium  $\kappa = 0$ ,  $n' = n_0$ . The resulting fields are (omitting the exponential factors for simplicity),

$$\vec{H} = n_o (-E_s \cos \phi \hat{x} + E_p \hat{y} + E_s \sin \phi \hat{z}) \quad (36)$$

$$\vec{H}'' = n_o (E_s'' \cos \phi \hat{x} - E_p'' \hat{y} + E_s'' \sin \phi \hat{z}) \quad (37)$$

$$\vec{H}' = n' (-E_s (\cos \phi_r + i\kappa') \hat{x} + E_p' (1 - \kappa'^2 + i2\kappa' \cos \phi_r) \hat{y} + E_s' \sin \phi_r \hat{z}) \quad (38)$$

Assuming no surface charges or currents, the boundary conditions at the interface are that the components of B and  $n_c^2 E$  normal to the boundary and the components of E and H parallel to the boundary be continuous.\*

These conditions are expressed as follows:

$$n_o^2 (\vec{E} + \vec{E}'') \cdot \hat{z} = n_c^2 \vec{E}' \cdot \hat{z} \quad (39)$$

$$(\vec{H} + \vec{H}'') \cdot \hat{z} = \vec{H}' \cdot \hat{z} \quad (40)$$

$$(\vec{E} + \vec{E}'') \times \hat{z} = \vec{E}' \times \hat{z} \quad (41)$$

$$(\vec{H} + \vec{H}'') \times \hat{z} = \vec{H}' \times \hat{z} \quad (42)$$

Substitution of Eqs. (28), (29) and (35) into (39) and evaluation at  $z = 0$  gives, when the common exponential factor is cancelled,

$$n_o^2 (-E_p \sin \phi + E_p'' \sin \phi) = n_c^2 (-E_p' \sin \phi_r)$$

or

$$n_o^2 \sin \phi (E_p - E_p'') = n_c^2 \sin \phi_r E_p'$$

applying Eq. (34),

$$n_o \sin \phi = n' \sin \phi_r$$

one has

$$n_o (E_p - E_p'') = \frac{n_c^2}{n'} E_p' \quad (43)$$

\*

These conditions can be derived mathematically from Maxwell's Equations ([1] pp. 388-390).



When Eqs. (28), (29), and (35) are evaluated at  $z = 0$  and substituted into Eq. (41), there results, when the common exponential factor is cancelled,

$$(-E_p \cos \phi \hat{y} + E_s \hat{x} - E_p'' \cos \phi \hat{y} + E_s'' \hat{x}) = [-E_p'(\cos \phi_r + i\kappa')\hat{y} + E_s' \hat{x}]$$

Collecting terms,

$$-(E_p + E_p'' \cos \phi \hat{y} + \hat{x}(E_s + E_s'')) = -E_p'(\cos \phi_r + i\kappa')\hat{y} + E_s' \hat{x}$$

Hence,

$$\cos \phi (E_p + E_p'') = E_p'(\cos \phi_r + i\kappa') \quad (44)$$

and

$$E_s + E_s'' = E_s' \quad (45)$$

When Eqs. (36), (37), and (38) are evaluated at  $z = 0$  and substituted into Eq. (42), and the common exponential factor is cancelled, there results

$$\begin{aligned} n_o (\hat{y} E_s \cos \phi + \hat{x} E_p - E_s'' \cos \phi \hat{y} - E_p'' \hat{x}) \\ = n' [\hat{y} E_s' (\cos \phi_r + i\kappa') + \hat{x} E_p' (1 - \kappa'^2 + 2i\kappa' \cos \phi_r)] \end{aligned}$$

or

$$\begin{aligned} n_o [(E_s - E_s'' \cos \phi \hat{y} + (E_p - E_p'') \hat{x}] = n' E_s' (\cos \phi_r + i\kappa') \hat{y} \\ + n' E_p' (1 - \kappa'^2 + 2i\kappa' \cos \phi_r) \hat{x} \end{aligned}$$

This last equation implies that

$$n_o (E_s - E_s'') \cos \phi = n' E_s' (\cos \phi_r + i\kappa') \quad (46)$$

$$n_o (E_p - E_p'') = n' E_p' (1 - \kappa'^2 + 2i\kappa' \cos \phi_r) \quad (47)$$

Equation (47) is the same as Eq. (43) since

$$n_c^2 = n'^2(1 - \kappa'^2) + 2in'\kappa' \cos \phi_r$$

by Eqs. (27a) and (27b).

To summarize, the boundary conditions have given the following four relations

$$n_o(E_p - E_p'') = \frac{n_c^2}{n'} E_p' \quad (43)$$

$$\cos \phi (E_p + E_p'') = E_p' (\cos \phi_r + i\kappa') \quad (44)$$

$$E_s + E_s'' = E_s' \quad (45)$$

$$n_o(E_s - E_s'') \cos \phi = n'E_s' (\cos \phi_r + i\kappa') \quad (46)$$

## 2. Derivation of Equations

In the calculations which follow, it will be useful to know the reflection coefficients at each interface. They are defined, in general, as

$$r_v \equiv \frac{E_{v\text{reflected}}}{E_{v\text{incident}}} \quad (48)$$

where  $v$  stands for either  $p$  or  $s$ .

The reflection coefficient for polarization normal to the plane of incidence,

$$r_s \equiv \frac{E_s''}{E_s'} \quad (49)$$

can be found from Eqs. (45) and (46).

From Eq. (45)

$$1 + \frac{E''_s}{E_s} = \frac{E'_s}{E_s} \quad (45a)$$

From Eq. (46)

$$\frac{E'_s}{E_s} = \frac{n_o \cos \phi}{n'(\cos \phi_r + i\kappa')} \left( 1 - \frac{E''_s}{E_s} \right) \quad (46a)$$

Equating (45a) and (46a),

$$1 + \frac{E''_s}{E_s} = \frac{n_o \cos \phi}{n'(\cos \phi_r + i\kappa')} \left( 1 - \frac{E''_s}{E_s} \right) \quad (50)$$

$$n'(\cos \phi_r + i\kappa') + n'(\cos \phi_r + i\kappa') \frac{E''_s}{E_s} = n_o \cos \phi - n_o \cos \phi \frac{E''_s}{E_s}$$

$$r_s \equiv \frac{E''_s}{E_s} = \frac{n_o \cos \phi - n'(\cos \phi_r + i\kappa')}{n_o \cos \phi + n'(\cos \phi_r + i\kappa')} \quad (51)$$

The reflection coefficient for polarization parallel to the plane of incidence,

$$r_p \equiv \frac{E''_p}{E_s} \quad (52)$$

is found from Eqs. (43) and (44) as follows:

First, divide Eq. (43) by  $E_p$  and multiply by  $n'/n_c^2$

$$\frac{n'n_o}{n_c^2} \left( 1 - \frac{E''_p}{E_p} \right) = \frac{E'_p}{E_p} \quad (43b)$$

Then divide Eq. (44) by  $E_p(\cos \phi_r + i\kappa')$

$$\frac{E'_p}{E_p} = \frac{\cos \phi}{\cos \phi_r + i\kappa'} \left( 1 + \frac{E''_p}{E_p} \right) \quad (44b)$$

Equating Eqs. (43b) and (44b),

$$\frac{n'_0}{n_c^2} \left( 1 - \frac{E''_p}{E_p} \right) = \frac{\cos \phi}{(\cos \phi_r + i\kappa')} \left( 1 + \frac{E''_p}{E_p} \right) \quad (52)$$

$$n'_0(\cos \phi_r + i\kappa') - n'_0(\cos \phi_r + i\kappa') \frac{E''_p}{E_p} = n_c^2 \cos \phi + n_c^2 \cos \phi \frac{E''_p}{E_p}$$

or

$$r_p \equiv \frac{E''_p}{E_p} = - \frac{n_c^2 \cos \phi - n'_0(\cos \phi_r + i\kappa')}{n_c^2 \cos \phi + n'_0(\cos \phi_r + i\kappa')} \quad (53)$$

E. Introduction of Complex Angle of Refraction and Formulation of the Fresnel Equations

Equations (51) and (53) can be written in a simpler form by defining the complex angle of refraction  $\phi'$ , by the complex form of Snell's Law.

$$n_0 \sin \phi = n' \sin \phi_r \equiv n_c \sin \phi' \quad (54)$$

This equation is consistent with the equation

$$n'(\cos \phi_r + i\kappa') = n_c \cos \phi' \quad (55)$$

as will now be demonstrated.

Squaring Eqs. (54) and (55) and adding, one has

$$\begin{aligned}
 n_c^2 &= n'^2 \sin^2 \phi_r + n'^2 (\cos \phi_r + i\kappa')^2 \\
 &= n'^2 (\sin^2 \phi_r + \cos^2 \phi_r) - n'^2 \kappa'^2 + n'^2 2i\kappa' \cos \phi_r \\
 n_c^2 &= n'^2 (1 - \kappa'^2) + i2n'^2 \kappa' \cos \phi_r \quad (56)
 \end{aligned}$$

But Eq. (56) is true because of Eqs. (27a) and (27b). Therefore, the consistency of Eq. (54) and (55) is established. Substituting Eq. (55) into Eq. (51) and (53), one has the Fresnel Equations

$$r_s = \frac{n_c \cos \phi - n_c \cos \phi'}{n_o \cos \phi + n_c \cos \phi'} \quad (57)$$

$$r_p = - \frac{n_c \cos \phi - n_o \cos \phi'}{n_c \cos \phi + n_o \cos \phi'} \quad (58)$$

Equation (54) will now be applied to (57) and (58) to arrive at alternate equations for  $r_s$  and  $r_p$ . In both Equations,  $n_c$  is replaced by

$$n_c = \frac{n_o \sin \phi}{\sin \phi'} \quad (54a)$$

First, considering Eq. (57),

$$\begin{aligned}
 r_s &= \frac{n_o \cos \phi - \frac{n_o \sin \phi}{\sin \phi'} \cos \phi'}{n_o \cos \phi + \frac{n_o \sin \phi \cos \phi'}{\sin \phi'}} \\
 &= \frac{\sin \phi' \cos \phi - \sin \phi \cos \phi'}{\sin \phi' \cos \phi + \sin \phi \cos \phi'} \\
 r_s &= - \frac{\sin (\phi - \phi')}{\sin (\phi + \phi')} \quad (59)
 \end{aligned}$$

Next, considering Eq. (58),

$$r_p = - \frac{n_o (\sin \phi / \sin \phi') \cos \phi - n_o \cos \phi'}{n_o (\sin \phi / \sin \phi') \cos \phi + n_o \cos \phi'}$$

$$= - \frac{\sin \phi \cos \phi - \sin \phi' \cos \phi'}{\sin \phi \cos \phi + \sin \phi' \cos \phi'}$$

divide top and bottom of the right side by  $\cos^2 \phi \cdot \cos^2 \phi'$

$$r_p = - \frac{\tan \phi / \cos^2 \phi' - \tan \phi' / \cos^2 \phi}{\tan \phi / \cos^2 \phi' + \tan \phi' / \cos^2 \phi}$$

$$= - \frac{\sec^2 \phi' \tan \phi - \sec^2 \phi \tan \phi'}{\sec^2 \phi' \tan \phi + \sec^2 \phi \tan \phi'}$$

$$= - \frac{(1 + \tan^2 \phi') \tan \phi - (1 + \tan^2 \phi) \tan \phi'}{(1 + \tan^2 \phi') \tan \phi + (1 + \tan^2 \phi) \tan \phi'}$$

$$= - \frac{\tan \phi + \tan \phi \tan^2 \phi' - \tan \phi' - \tan \phi' \tan^2 \phi}{\tan \phi + \tan \phi \tan^2 \phi' + \tan \phi' + \tan \phi' \tan^2 \phi}$$

$$= - \frac{(\tan \phi - \tan \phi') (1 - \tan \phi \tan \phi')}{(\tan \phi + \tan \phi') (1 + \tan \phi \tan \phi')}$$

$$= - \frac{(\tan \phi - \tan \phi') (1 + \tan \phi \tan \phi')}{(\tan \phi + \tan \phi') (1 - \tan \phi \tan \phi')}$$

$$r_p = - \frac{\tan (\phi - \phi')}{\tan (\phi + \phi')} \tag{60}$$

F. Summary

With the definitions

$$n_c \equiv \sqrt{\mu(\epsilon + i 4\pi\sigma/\omega)} \equiv n(1 + i\kappa) \quad (13), (14)$$

$$n'_c \equiv n'(1 + i\kappa')$$

$$n' \equiv c/v \quad (20)$$

$$\kappa' \equiv \alpha c/\omega n', \quad \alpha = \text{absorption coefficient} \quad (22)$$

and the relations

$$n^2(1 - \kappa^2) = n'^2(1 - \kappa'^2) \quad (27a)$$

$$n^2\kappa = n'^2\kappa' \cos \phi_r \quad (27b)$$

$$n_o \sin \phi = n' \sin \phi_r \quad (34)$$

The reflection coefficients can be written

$$r_s = \frac{n_o \cos \phi - n'(\cos \phi_r + i\kappa')}{n_o \cos \phi + n'(\cos \phi_r + i\kappa')} \equiv \frac{E_s \text{ reflected}}{E_s \text{ incident}} \quad (51)$$

$$r_p = -\frac{n_c^2 \cos \phi - n_o n'(\cos \phi_r + i\kappa')}{n_c^2 \cos \phi + n_o n'(\cos \phi_r + i\kappa')} \equiv \frac{E_p \text{ reflected}}{E_p \text{ incident}} \quad (53)$$

With the additional definition of the complex angle of refraction  $\phi'$

$$n' \sin \phi_r \equiv n_c \sin \phi' \quad (54)$$

and the auxiliary equation

$$n'(\cos \phi_r + i\kappa') = n_c \cos \phi' \quad (55)$$

The Fresnel equations can be written

$$r_s = \frac{n_o \cos \phi - n_c \cos \phi'}{n_o \cos \phi + n_c \cos \phi'} = - \frac{\sin (\phi - \phi')}{\sin (\phi + \phi')} \quad (57), (59)$$

$$r_p = \frac{n_o \cos \phi' - n_c \cos \phi}{n_o \cos \phi' + n_c \cos \phi} = - \frac{\tan (\phi - \phi')}{\tan (\phi + \phi')} \quad (58), (60)$$

Equations (51), (53), (57), (58), (59), and (60) assume that the incident medium is transparent (i.e., of zero conductivity).

Better suited for numerical purposes are the equations summarized in sections IIIf and IIIId as they contain all real quantities.



## CHAPTER II

OPTICAL CONSTANTS  $n$ ,  $\kappa$  AND ELLIPSOMETRIC PARAMETERS  $\Delta$ ,  $\psi$ A. Introduction and Definition of  $\Delta$ ,  $\psi$ 

When polarized light is reflected from a metallic surface, the components of the electric field parallel and normal to the plane of incidence undergo an unequal amplitude attenuation, and a phase difference  $\Delta$  is introduced between them. When the electric field components are  $E_p$  and  $E_s$  before reflection, and  $E_p''$  and  $E_s''$  after reflection, then the ratios of s and p amplitudes in the incident and reflected light are defined by

$$\tan \psi_i \equiv \frac{|E_s|}{|E_p|} \quad (61)$$

$$\tan \psi_r \equiv \frac{|E_s''|}{|E_p''|} \quad (62)$$

Thus, the amplitude ratio is changed on reflection by the factor

$$\tan \psi \equiv \frac{\tan \psi_r}{\tan \psi_i} \quad (63)$$

$\tan \psi$  is the relative amplitude attenuation due to reflection. Figure 2 illustrates the coordinate system to be used. The x-z plane is the plane of incidence. The x-y plane defines the surface at which reflection and refraction occur. Figure 3 shows the relation of the magnetic and electric field vectors for the cases of polarization parallel (Fig. 3a) and normal (Fig. 3b) to the plane of incidence.

In this section, light will be incident from a medium of real refractive index  $n_0$  onto the plane surface of a metal of complex

refractive index

$$n_c = n(1 + i\kappa) \text{ or } n'_c = n'(1 + i\kappa')$$

defined as in Chapter I.

The ratios  $E''_s/E_s$  and  $E''_p/E_p$  are related to the angles of incidence and refraction by the Fresnel Equations

$$r_s \equiv \frac{E''_s}{E_s} = - \frac{\sin(\phi - \phi')}{\sin(\phi + \phi')} \quad (59)$$

$$r_p \equiv \frac{E''_p}{E_p} = - \frac{\tan(\phi - \phi')}{\tan(\phi + \phi')} \quad (60)$$

The quantities  $r_s$  and  $r_p$  are called the reflection coefficients of the surface, and  $\phi'$  is the complex angle of refraction introduced in Chapter I Section E.

The reflection coefficients are, in general, complex, so that they can be written as an amplitude ratio and a phase change

$$r_s = \frac{E''_s}{E_s} = \frac{|E''_s|}{|E_s|} \frac{e^{-i\epsilon''_s}}{e^{-i\epsilon_s}} = \frac{|E''_s|}{|E_s|} e^{-i(\epsilon''_s - \epsilon_s)} \quad (59a)$$

$$r_p = \frac{E''_p}{E_p} = \frac{|E''_p|}{|E_p|} \frac{e^{-i\epsilon''_p}}{e^{-i\epsilon_p}} = \frac{|E''_p|}{|E_p|} e^{-i(\epsilon''_p - \epsilon_p)} \quad (60a)$$

where the epsilons are the phases of the various components with respect to an arbitrary time origin. If we define the "absolute" phase changes of the reflected with respect to incident waves as

$$\delta_s \equiv \epsilon''_s - \epsilon_s, \quad \delta_p \equiv \epsilon''_p - \epsilon_p, \quad (64)$$

where p refers to polarization parallel and s to polarization perpendicular to the plane of incidence, then the ratio of the reflection coefficients is

$$\rho \equiv \frac{r_s}{r_p} = \left( \frac{|E_s''|}{|E_s|} / \frac{|E_p''|}{|E_p|} \right) \frac{e^{-i\delta_s}}{e^{-i\delta_p}} \quad (65)$$

$$\rho = \left( \frac{|E_s''|}{|E_p''|} / \frac{|E_s|}{|E_p|} \right) e^{i(\delta_p - \delta_s)}$$

which equals, using Eqs. (61) and (62),

$$\rho = \frac{\tan \psi_r}{\tan \psi_i} e^{i(\delta_p - \delta_s)} \quad (65a)$$

But  $\delta_p - \delta_s$  is the phase difference imposed between the p and s components on reflection. Thus, defining the relative phase change as

$$\Delta \equiv \delta_p - \delta_s \quad (66)$$

and using Eq. (63) one has

$$\rho = \tan \psi e^{i\Delta} \quad (67)$$

A word is in order concerning the definitions (64). Consider a harmonic oscillator vibrating with frequency  $\omega$  and relative phase  $\theta$ , represented in complex notation by  $e^{-i(\omega t + \theta)}$ . Figure 4b shows the oscillation in the complex plane. As time increases, the rotation of the radius vector proceeds clockwise. Suppose that at  $t = t_0$  the phase of the oscillation is suddenly changed by reflection so that before the change it is  $\theta_1$ , and after the change it is  $\theta_2$ , the phase change being defined as  $\theta_2 - \theta_1$ . When  $\theta_2$  is larger than  $\theta_1$ , the total argument  $\omega t_0 + \theta_2$  is greater than the total argument  $\omega t_0 + \theta_1$  before the change and is equivalent to holding  $\theta_1$  constant and increasing  $t$ . That is, a positive phase change  $\theta_2 - \theta_1$  is equivalent to an advance in time.

Therefore, with the definitions chosen in (64), a positive phase change

$\theta_2 - \theta_1$  is equivalent to an advance in time.\*

### B. Derivation of Equations

Equation (67) is the basic equation of ellipsometry. The quantities  $\psi$  and  $\Delta$ , which are parameters used to describe the relation between the polarization states of the light before and after reflection, can be found from ellipsometer measurements [10]. The equations relating  $\psi$  and  $\Delta$  to the optical constants  $n$  and  $\kappa$  which characterize the reflecting surface will now be derived.

By Eqs. (59) and (60),

$$\rho = \frac{r_s}{r_p} = \frac{\sin(\phi - \phi')}{\sin(\phi + \phi')} \bigg/ \frac{\tan(\phi - \phi')}{\tan(\phi + \phi')} \quad (68)$$

$$\rho = \frac{\cos(\phi - \phi')}{\cos(\phi + \phi')} = \tan \psi e^{i\Delta} \quad (69)$$

rewriting Eq. (69),

$$1 - \tan \psi e^{i\Delta} = 1 - \frac{\cos \phi \cos \phi' + \sin \phi \sin \phi'}{\cos \phi \cos \phi' - \sin \phi \sin \phi'}$$

$$1 - \tan \psi e^{i\Delta} = \frac{\cos \phi \cos \phi' - \sin \phi \sin \phi' - \cos \phi \cos \phi' - \sin \phi \sin \phi'}{\cos \phi \cos \phi' - \sin \phi \sin \phi'} \quad (70)$$

Similarly,

$$1 + \tan \psi e^{i\Delta} = \frac{\cos \phi \cos \phi' - \sin \phi \sin \phi' + \cos \phi \cos \phi' + \sin \phi \sin \phi'}{\cos \phi \cos \phi' - \sin \phi \sin \phi'} \quad (71)$$

dividing Eq. (71) by Eq. (70) leaves

---

\* See Appendix I for a discussion of alternate representations of the phase of a harmonic oscillation.

$$\frac{1 + \tan\psi e^{i\Delta}}{1 - \tan\psi e^{i\Delta}} = - \frac{\cos\phi \cos\phi'}{\sin\phi \sin\phi'} \quad (72)$$

The left side of Eq. (72) can be rewritten as

$$\begin{aligned} \frac{1 + \tan\psi e^{i\Delta}}{1 - \tan\psi e^{i\Delta}} &= \frac{1 + (\sin\psi/\cos\psi) e^{i\Delta}}{1 - (\sin\psi/\cos\psi) e^{i\Delta}} \\ &= \frac{\cos\psi + (\cos\Delta + i \sin\Delta) \sin\psi}{\cos\psi - (\cos\Delta + i \sin\Delta) \sin\psi} \\ &= \frac{(\cos\psi + \cos\Delta \sin\psi) + i \sin\Delta \sin\psi}{(\cos\psi - \cos\Delta \sin\psi) - i \sin\Delta \sin\psi} \end{aligned}$$

$$= \left[ \frac{(\cos\psi + \cos\Delta \sin\psi) + i \sin\Delta \sin\psi}{(\cos\psi - \cos\Delta \sin\psi) - i \sin\Delta \sin\psi} \right] \cdot \left[ \frac{(\cos\psi - \cos\Delta \sin\psi) + i \sin\Delta \sin\psi}{(\cos\psi - \cos\Delta \sin\psi) + i \sin\Delta \sin\psi} \right]$$

$$= \frac{\cos^2\psi - \cos^2\Delta \sin^2\psi - \sin^2\Delta \sin^2\psi + i \sin\Delta \sin\psi (\cos\psi + \cos\Delta \sin\psi + \cos\psi - \cos\Delta \sin\psi)}{(\cos\psi - \cos\Delta \sin\psi)^2 + \sin^2\Delta \sin^2\psi}$$

$$= \frac{\cos^2\psi - \sin^2\psi (\sin^2\Delta + \cos^2\Delta) + i 2 \sin\psi \cos\psi \sin\Delta}{\cos^2\psi + \cos^2\Delta \sin^2\psi - \cos\Delta 2\cos\psi \sin\psi + \sin^2\Delta \sin^2\psi}$$

Finally,

$$\frac{1 + \tan\psi e^{i\Delta}}{1 - \tan\psi e^{i\Delta}} = \frac{\cos 2\psi + i \sin 2\psi \sin\Delta}{1 - \sin 2\psi \cos\Delta} \quad (73)$$

With Eq. (73), Eq. (72) becomes

$$\frac{\cos 2\psi + i \sin 2\psi \sin\Delta}{1 - \sin 2\psi \cos\Delta} = - \frac{\cos\phi \cos\phi'}{\sin\phi \sin\phi'} \quad (74)$$

Define a and b by the equation

$$n_c \cos \phi' = n'(\cos \phi_r + i\kappa') \equiv a + ib \quad (75)$$

Since  $0 \leq \phi_r \leq 90$ ,  $\cos \phi_r$  is real and positive. Also  $n'$  and  $\kappa'$  are real and positive by definition. Therefore, by Eq. (75)  $a$  and  $b$  must be real and positive.

With the aid of Eqs. (54) and (75), Eq. (74) becomes

$$\frac{\cos 2\psi}{1 - \sin 2\psi \cos \Delta} + i \frac{\sin 2\psi \sin \Delta}{1 - \sin \psi^2 \cos \Delta} = - \frac{(a + ib)}{n_o \sin \phi \tan \phi} \quad (76)$$

Equating real parts of Eq. (76)

$$a = - \frac{n_o \sin \phi \tan \phi \cos 2\psi}{1 - \sin \psi^2 \cos \Delta} \quad (77)$$

A very important fact is contained in Eq. (77). Since the angle of incidence  $\phi$  must be in the range  $0 \leq \phi \leq 90$ ,  $\sin \phi$  and  $\tan \phi$  are positive. Furthermore, the denominator of Eq. (77) is positive because the product of a sine and cosine can never exceed unity. Also  $n_o$  is positive by definition. Therefore, in order that the right side of Eq. (77) be positive as required by Eq. (75),  $\cos 2\psi$  must be negative, which would mean that  $\psi$  lies between  $45^\circ$  and  $135^\circ$ . However, for the most general use of elliptic polarization  $\psi$  has been found [10] to lie in the interval  $0 \leq \psi \leq 90^\circ$  under the conventions employed here. Therefore, for reflection from a metal surface:

$$45^\circ \leq \psi \leq 90^\circ . \quad (78)$$

Equating imaginary parts of Eq. (76)

$$b = - \frac{n_o \sin\phi \tan\phi \sin 2\psi \sin\Delta}{1 - \sin 2\psi \cos\Delta} \quad (79)$$

There is also an important result contained in Eq. (79). Applying the same type of argument used to establish Eq. (78) to Eq. (79), one finds that  $\sin\Delta$  has to be negative; therefore, the relative phase change  $\Delta$  must lie in the range

$$-\pi \leq \Delta \leq 0 \quad (80)$$

or equivalently

$$\pi \leq \Delta \leq 2\pi, \text{ etc.}$$

The index of the incident (transparent) medium can be eliminated from the following equations by introducing A and B defined as

$$A \equiv a/n_o = - \frac{\sin\phi \tan\phi \cos 2\psi}{1 - \sin 2\psi \cos\Delta} \quad (81)$$

$$B \equiv b/n_o = - \frac{\sin\phi \tan\phi \sin 2\psi \sin\Delta}{1 - \sin 2\psi \cos\Delta} \quad (82)$$

It is now possible to obtain explicit expressions for  $n'$  and  $\kappa'$  in terms of the measured parameters  $\phi$ ,  $\psi$ , and  $\Delta$ . The real part of Eq. (75) can be rewritten, with the aid of Eq. (34),

$$\cos \phi_r = \sqrt{1 - \sin^2 \phi_r} = \sqrt{1 - \frac{n_o^2 \sin^2 \phi}{n'^2}}$$

as

$$n'^2 \cos^2 \phi_r = a^2 = n'^2 - n_o^2 \sin^2 \phi$$

$$n' = + \sqrt{a^2 + n_o^2 \sin^2 \phi} = n_o \sqrt{A^2 + \sin^2 \phi} \quad (83)$$

Since  $n'$  is defined as the ratio of light propagation rates, it must be a positive quantity. Therefore, the positive square root is taken in Eq. (83). Alternatively, Eq. (83a) is obtained from Eq. (83) by substituting  $A$  from Eq. (81).

$$n' = n_o \sin \phi \left[ 1 + \frac{\tan^2 \phi \cos^2 2\psi}{(1 - \sin 2\psi \cos \Delta)^2} \right]^{1/2} \quad (83a)$$

The imaginary part of Eq. (75) can be written as

$$\kappa' = \frac{b}{n'}$$

Substituting from Eq. (79) and Eq. (83a),

$$\kappa' = \frac{-n_o \sin \phi \tan \phi \sin 2\psi \sin \Delta}{1 - \sin 2\psi \cos \Delta} \cdot n_o \sin \phi \left[ 1 + \frac{\tan^2 \phi \cos^2 2\psi}{(1 - \sin 2\psi \cos \Delta)^2} \right]^{1/2}$$

or

$$\kappa' = \frac{-\tan \phi \sin 2\psi \sin \Delta}{\sqrt{(1 - \sin 2\psi \cos \Delta)^2 + \tan^2 \phi \cos^2 2\psi}} \quad (84)$$

As defined in Chapter I, Eq. (22a)

$$\kappa' = \frac{\lambda_o \alpha}{2\pi n'}$$

where  $\alpha$  is the absorption coefficient.

Since  $\alpha$  and  $n'$  are positive,  $\kappa'$  must also be positive. Since  $\sin \Delta$  is negative and  $\tan \phi$  and  $\sin 2\psi$  are positive, the positive square



root is taken in Eq. (84).

It is also possible to find explicit expressions for  $n$  and  $\kappa$ .

Square Eq. (75) to obtain

$$(a + ib)^2 = n_c^2 \cos^2 \phi' = n_c^2 (1 - \sin^2 \phi') = n_c^2 - n_c^2 \sin^2 \phi' = n_c^2 - n_o^2 \sin^2 \phi$$

where the last step is made with the use of Eq. (54).

Next, expand  $(a + ib)^2$ ,

$$\begin{aligned} a^2 - b^2 + 2iab &= n_c^2 - n_o^2 \sin^2 \phi \\ &= n^2(1 + i\kappa)^2 - n_o^2 \sin^2 \phi \\ &= n^2(1 - \kappa^2 + 2i\kappa) - n_o^2 \sin^2 \phi \\ \therefore a^2 - b^2 + 2abi &= n^2(1 - \kappa^2) - n_o^2 \sin^2 \phi + 2in^2\kappa \end{aligned} \quad (85)$$

Equate real parts of Eq. (85) to get

$$a^2 - b^2 = n^2(1 - \kappa^2) - n_o^2 \sin^2 \phi \quad (86)$$

Equate imaginary parts of Eq. (85) to get

$$n^2 \kappa = ab \quad (87)$$

Equations (86) and (87) can now be solved for  $n$  and  $\kappa$  in terms of  $a$ ,  $b$ , and  $\phi$ . From Eq. (86),

$$n^2 = \frac{a^2 - b^2 + n_o^2 \sin^2 \phi}{(1 - \kappa^2)} \quad (86a)$$

inserting  $\kappa$  from Eq. (87) into Eq. (86) yields

$$n^2 = \frac{a^2 - b^2 + n_o^2 \sin^2 \phi}{1 - a^2 b^2 / n^4}$$

$$= \frac{n^4 (a^2 - b^2 + n_o^2 \sin^2 \phi)}{n^4 - a^2 b^2}$$

$$n^2 (n^4 - a^2 b^2) = n^4 (a^2 - b^2 + n_o^2 \sin^2 \phi)$$

$$n^4 - n^2 (a^2 - b^2 + n_o^2 \sin^2 \phi) - a^2 b^2 = 0 \quad (87a)$$

Equation (87a) can be solved for  $n^2$  by the quadratic formula. This results in agreement with Konig [3].\*

$$n^2 = \frac{1}{2} [(a^2 - b^2 + n_o^2 \sin^2 \phi) + \sqrt{(a^2 - b^2 + n_o^2 \sin^2 \phi)^2 + 4a^2 b^2}] \quad (88)$$

Since  $n$  is real by definition,  $n^2$  is positive. The second term in the bracket is larger than the first, therefore the positive sign has to be used for the square root in Eq. (88).

A similar expression for  $\kappa$  will now be obtained. Again, from Eq. (84),

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\* It should be noted that Konig's  $\psi$  is the complement of the  $\psi$  defined by Eq. (63). In addition, his  $\rho$  is the inverse of the  $\rho$  given by Eq. (67). Thus, his  $\Delta$  is the same as ours. A further difference is that with Konig the time variation of the electric and magnetic fields is formulated as  $e^{+i\omega t}$  while here it is  $e^{-i\omega t}$ .

$$n^2(1 - \kappa^2) = a^2 - b^2 + n_o^2 \sin^2 \phi$$

by Eq. (85)

$$n^2 = \frac{ab}{\kappa}$$

Thus,

$$\frac{ab}{\kappa} (1 - \kappa^2) = a^2 - b^2 + n_o^2 \sin^2 \phi$$

$$ab(1 - \kappa^2) = \kappa(a^2 - b^2 + n_o^2 \sin^2 \phi)$$

$$\kappa^2 + \frac{\kappa}{ab} (a^2 - b^2 + n_o^2 \sin^2 \phi) - 1 = 0 \quad (89)$$

Equation (89) is also of the quadratic form. The solution for  $\kappa$  is

$$\kappa = \frac{1}{2ab} \left[ \pm \sqrt{(a^2 - b^2 + n_o^2 \sin^2 \phi)^2 + 4a^2 b^2} - (a^2 - b^2 + n_o^2 \sin^2 \phi) \right] \quad (90)$$

The ambiguities in sign in Eq. (90) and in Eq. (91) below will be discussed later.

Equation (90) can be manipulated to give an expression presented by Konig for  $\kappa^2$  as follows.

From Eq. (85),

$$2ab = 2n^2 \kappa$$

Thus, Eq. (90) can be written

$$\kappa = \frac{1}{2n^2 \kappa} \left[ \pm \sqrt{(a^2 - b^2 + n_o^2 \sin^2 \phi)^2 + 4a^2 b^2} - (a^2 - b^2 + n_o^2 \sin^2 \phi) \right]$$

or

$$\kappa^2 = \frac{1}{2n^2} \left[ \pm \sqrt{(a^2 - b^2 + n_o^2 \sin^2 \phi)^2 + 4a^2 b^2} - (a^2 - b^2 + n_o^2 \sin^2 \phi) \right]$$

Substituting the value of  $2n^2$  from Eq. (88),

$$\kappa^2 = \frac{\pm \sqrt{(a^2 - b^2 + n_o^2 \sin^2 \phi)^2 + 4a^2 b^2} - (a^2 - b^2 + n_o^2 \sin^2 \phi)}{\pm \sqrt{(a^2 - b^2 + n_o^2 \sin^2 \phi)^2 + 4a^2 b^2} + (a^2 - b^2 + n_o^2 \sin^2 \phi)} \quad (91)$$

If one defines the quantities

$$A \equiv a/n_o = - \frac{\sin \phi \tan \phi \cos 2\psi}{1 - \sin 2\psi \cos \Delta} \quad (81)$$

$$B \equiv b/n_o = - \frac{\sin 2\psi \sin \phi \tan \phi \sin \Delta}{1 - \sin 2\psi \cos \Delta} \quad (82)$$

$$N \equiv n/n_o \quad (92)$$

Equations (88) and (91) can be written

$$n^2 = (n_o^2/2)(A^2 - B^2 + \sin^2 \phi + \sqrt{(A^2 - B^2 + \sin^2 \phi)^2 + 4A^2 B^2}) \quad (88a)$$

$$\kappa^2 = \frac{\pm \sqrt{(A^2 - B^2 + \sin^2 \phi)^2 + 4A^2 B^2} - (A^2 - B^2 + \sin^2 \phi)}{\pm \sqrt{(A^2 - B^2 + \sin^2 \phi)^2 + 4A^2 B^2} + A^2 - B^2 + \sin^2 \phi} \quad (91a)$$

and Eqs. (85) and (90) become

$$n = n_o \sqrt{\frac{AB}{\kappa}}$$

or

$$N = \sqrt{\frac{AB}{\kappa}} \quad (85a)$$

$$\kappa = \frac{1}{2AB} [\pm \sqrt{(A^2 - B^2 + \sin^2 \phi)^2 + 4A^2 B^2} - (A^2 - B^2 + \sin^2 \phi)] \quad (90a)$$

C. Discussion of Signs of  $n, \kappa$

The ambiguity of sign in Eqs. (90) and (91) will now be resolved.

Since  $\sqrt{(a^2 - b^2 + n_o^2 \sin^2 \phi)^2 + 4a^2 b^2}$  is generally larger than  $(a^2 - b^2 + n_o^2 \sin^2 \phi)$ , and since  $a$  and  $b$  are positive and  $\kappa^2$  must be positive, the positive square root must be taken in Eq. (90). Thus the positive square root is taken also in the numerators of Eqs. (91) and (91a). Since  $\kappa^2$  must be positive and the numerators are positive, the denominators of (91) and (91a) must be positive also. Hence, the positive square roots are taken in Eqs. (91) and (91a).

As mentioned in the last section,  $n'$  and  $\kappa'$  must be positive.

Since the real angle of refraction  $\phi_r$  is never greater than  $90^\circ$  and is never negative,  $\cos \phi_r \geq 0$ . The quantities  $n$  and  $n'$  are real so  $n^2$  and  $n'^2$  must be positive.

Therefore, Eq. (27b)

$$n^2 \kappa = + n'^2 \kappa' \cos \phi_r \quad (27b)$$

implies that

$$\kappa \geq 0$$

So, once  $\kappa^2$  is found from Eqs. (91) or (91a),  $\kappa$  is found by taking the positive square root.

The sign of  $n$  can be determined from Eqs. (54) and (55),

$$n' \sin \phi_r = n_c \sin \phi' \quad (54)$$

$$n'(\cos \phi_r + i\kappa') = n_c \cos \phi' \quad (55)$$

Equation (54) implies that  $n_c$  and  $\sin \phi'$  have the same sign, since  $n' \sin \phi_r$

is positive.

It follows that if  $n_c$  is negative,  $\phi'$  is negative, and  $\cos\phi'$  is positive. Then in Eq. (55), either  $n'$  or  $\cos\phi_r + i\kappa'$  must be negative. But it has already been shown that these three quantities are all positive. Therefore,  $n_c$  cannot be negative. It follows that  $n$  cannot be negative, and the positive square root must be taken in Eqs. (88) or (88a).

D. Summary (Determination of Optical Constants From Ellipse Parameters)

Ellipsometric measurements are converted to values of  $\Delta$  and  $\psi$ .<sup>10</sup> Then,  $\Delta$ ,  $\psi$ , and  $\phi$  are used to find the intermediate variables A and B from

$$A = - \frac{\sin\phi \tan\phi \cos 2\psi}{1 - \sin 2\psi \cos\Delta} \quad (81)$$

$$B = - \frac{\sin 2\psi \sin\phi \tan\phi \sin\Delta}{1 - \sin 2\psi \cos\Delta} \quad (82)$$

Next the optical constants  $n$  and  $\kappa$  of the complex refractive index  $n(1+i\kappa)$  are found from

$$n^2 = \frac{n_o^2}{2} (A^2 - B^2 + \sin^2\phi + \sqrt{(A^2 - B^2 + \sin^2\phi)^2 + 4A^2B^2}) \quad (88a)$$

$$\kappa^2 = \frac{+ \sqrt{(A^2 - B^2 + \sin^2\phi)^2 + 4A^2B^2} - (A^2 - B^2 + \sin^2\phi)}{+ \sqrt{(A^2 - B^2 + \sin^2\phi)^2 + 4A^2B^2} + A^2 - B^2 + \sin^2\phi} \quad (91a)$$

$$n, \kappa \geq 0$$

Or, one can find  $\kappa$  from

$$\kappa = \frac{1}{2AB} \left[ + \sqrt{(A^2 - B^2 + \sin^2 \phi)^2 + 4A^2 B^2} - (A^2 - B^2 + \sin^2 \phi) \right] \quad (90a)$$

and  $n$  from

$$n = +n_0 \sqrt{\frac{AB}{\kappa}} \quad (84)$$

Alternatively  $n'$  and  $\kappa'$  can be found directly from  $\Delta$ ,  $\psi$ , and  $\phi$  by using

$$n' = n_0 \sin \phi \left[ 1 + \frac{\tan^2 \phi \cos^2 2\psi}{(1 - \sin 2\psi \cos \Delta)^2} \right]^{1/2} \quad (83a)$$

and

$$\kappa' = \frac{-\tan \phi \sin 2\psi \sin \Delta}{\sqrt{(1 - \sin 2\psi \cos \Delta)^2 + \tan^2 \phi \cos^2 2\psi}} \quad (84)$$

The positive square root is to be taken in Eq. (83a).

In these equations  $n'$  is the ratio of the (real) phase velocity of light in the medium to that in vacuum,  $\kappa'$  is directly related to the absorption coefficient  $\alpha$  by  $\alpha = \frac{n' \kappa' \omega}{c}$ . The quantities  $n$  and  $\kappa$  can be related directly to the conductivity and dielectric constants (both real) of the medium through Eqs. (13) and (14).

A FORTRAN computer program (named MOC) is given in Chapter IV, Section A1, to determine the metal optical constants  $n$  and  $\kappa$  from measured values of  $\psi$ ,  $\Delta$  and  $\phi$ , by use of Eqs. (81), (82), (88a), and (91a). A second program (named AUXCON) given in Chapter IV, Section A2, can be used to find the metal optical constants  $n$  and  $\kappa$ , the auxiliary constants  $n'$  and  $\kappa'$ , the electrical constants  $\sigma$  (conductivity) and  $\epsilon$  (dielectric

constant), and the penetration depth from given values of  $\psi$ ,  $\Delta$  and  $\phi$ .

#### E. Determination of $\psi$ and $\Delta$ from $n$ and $\kappa$

Equations (81), (82), (88a) and (91a) allow one to calculate the optical constants  $n$  and  $\kappa$  from measured values of  $\phi$ ,  $\Delta$ , and  $\psi$ . Inverse equations will now be derived<sup>3, 14</sup> which allow calculation of  $\psi$  and  $\Delta$  from known values of  $n$  and  $\kappa$ .

The first thing to do is to get  $A$  and  $B$  in terms of  $N$ ,  $\kappa$ , and  $\phi$ . The starting point is Eq. (75)

$$n_c \cos \phi' = \sqrt{n_c^2 - n_o^2 \sin^2 \phi} = a + ib \quad (75)$$

When Eq. (75) is multiplied by its complex conjugate, one obtains

$$(a-ib)(a+ib) = \sqrt{n^2(1-i\kappa)^2 - n_o^2 \sin^2 \phi} \sqrt{n^2(1+i\kappa)^2 - n_o^2 \sin^2 \phi}$$

$$a^2 + b^2 = \sqrt{[n^2(1-\kappa^2) - n_o^2 \sin^2 \phi - 2in^2\kappa][n^2(1-\kappa^2) - n_o^2 \sin^2 \phi + 2in^2\kappa]}$$

$$a^2 + b^2 = \sqrt{[n^2(1-\kappa^2) - n_o^2 \sin^2 \phi]^2 + 4n^4 \kappa^2} \quad (104)$$

In addition, one also has Eq. (86),

$$a^2 - b^2 = n^2(1 - \kappa^2) - n_o^2 \sin^2 \phi$$

From Eqs. (86) and (104)

$$a^2 = \frac{1}{2} \left[ + \sqrt{[n^2(1-\kappa^2) - n_o^2 \sin^2 \phi]^2 + 4n^4 \kappa^2} + n^2(1-\kappa^2) - n_o^2 \sin^2 \phi \right] \quad (105)$$



$$b^2 = \frac{1}{2} \left[ \sqrt{[n^2(1-\kappa^2) - n_o^2 \sin^2 \phi]^2 + 4n^4 \kappa^2} - n^2(1-\kappa^2) + n_o^2 \sin^2 \phi \right] \quad (106)$$

Take the positive square roots of Eqs. (105) and (106) to get a and b.

With

$$A \equiv a/n_o \quad (81)$$

$$B \equiv b/n_o \quad (82)$$

$$N \equiv n/n_o \quad (92)$$

Equations (105) and (106) can be written

$$A^2 = \frac{1}{2} \sqrt{[N^2(1-\kappa^2) - \sin^2 \phi]^2 + 4N^4 \kappa^2} + N^2(1-\kappa^2) - \sin^2 \phi \quad (107)$$

Take the positive square root of Eq. (107) to get A.

$$B^2 = \frac{1}{2} \sqrt{[N^2(1-\kappa^2) - \sin^2 \phi]^2 + 4N^4 \kappa^2} - N^2(1-\kappa^2) + \sin^2 \phi \quad (108)$$

Take the positive square root of Eq. (108) to get B.

An equation giving  $\tan \Delta$  as a function of A, B, and  $\phi$  can be found as follows. Returning to Eq. (69),

$$\begin{aligned} \tan \psi e^{i\Delta} &= \frac{\cos(\phi - \phi')}{\cos(\phi + \phi')} \\ &= \frac{\cos \phi \cos \phi' + \sin \phi \sin \phi'}{\cos \phi \cos \phi' - \sin \phi \sin \phi'} \end{aligned}$$

Substituting from Eqs. (54) and (75) this becomes

$$\tan \psi e^{i\Delta} = \frac{\cos \phi \left( \frac{a+ib}{n_c} \right) + \sin \phi \frac{n_o \sin \phi}{n_c}}{\cos \phi \left( \frac{a+ib}{n_c} \right) - \sin \phi \frac{n_o \sin \phi}{n_c}}$$

Multiply the top and bottom of the right side by  $n_c/n_o$  and use Eqs. (81) and (82) to get

$$\begin{aligned} \tan\psi e^{i\Delta} &= \frac{(A + iB) \cos\phi + \sin\phi \sin\phi}{(A + iB) \cos\phi - \sin\phi \sin\phi} \\ &= \frac{A + iB + \sin\phi \tan\phi}{A + iB - \sin\phi \tan\phi} \\ &= \frac{A + \sin\phi \tan\phi + iB}{A - \sin\phi \tan\phi + iB} \end{aligned} \quad (109)$$

$$\begin{aligned} \tan\psi (\cos\Delta + i \sin\Delta) &= \frac{(A + \sin\phi \tan\phi + iB)(A - \sin\phi \tan\phi - iB)}{(A - \sin\phi \tan\phi + iB)(A - \sin\phi \tan\phi - iB)} \\ &= \frac{A^2 + B^2 - \sin^2\phi \tan^2\phi - 2iB\sin\phi \tan\phi}{A^2 + B^2 - 2A\sin\phi \tan\phi + \sin^2\phi \tan^2\phi} \end{aligned}$$

Equating the real and imaginary parts one has

$$\tan\psi \cos\Delta = \frac{A^2 + B^2 - \sin^2\phi \tan^2\phi}{A^2 + B^2 - 2A \sin\phi \tan\phi + \sin^2\phi \tan^2\phi} \quad (110)$$

and

$$\tan\psi \sin\Delta = - \frac{2B \sin\phi \tan\phi}{A^2 + B^2 - 2A \sin\phi \tan\phi + \sin^2\phi \tan^2\phi} \quad (111)$$

Dividing Eq. (111) by Eq. (110) leaves

$$\tan\Delta = - \frac{2B \sin\phi \tan\phi}{A^2 + B^2 - \sin^2\phi \tan^2\phi} \quad (112)$$

Two other quantities of interest are the reflectivities of the surface. These are the moduli of the reflection coefficients. Returning

to Eq. (59),

$$r_s = - \frac{\sin(\phi - \phi')}{\sin(\phi + \phi')} \quad (59)$$

one may write

$$r_s = \frac{\sin\phi' \cos\phi - \sin\phi \cos\phi'}{\sin\phi' \cos\phi + \sin\phi \cos\phi'}$$

$$= \frac{\frac{n_o \sin\phi}{n_c} \cos\phi - \sin\phi \frac{(a+ib)}{n_c}}{\frac{n_o \sin\phi}{n_c} \cos\phi + \sin\phi \frac{(a+ib)}{n_c}}$$

Multiply the numerator and denominator by  $n_c/n_o$  and use Eqs. (81) and (82)

to get

$$r_s = \frac{\cos\phi - A - iB}{\cos\phi + A + iB}$$

If one defines <sup>\*\*</sup> the reflectivity  $R_s$  as the modulus of the reflection coefficient,  $r_s$ , i.e.

$$r_s r_s^* \equiv R_s^2$$

where  $r_s^*$  is the complex conjugate of the Fresnel coefficient  $r_s$ , then

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<sup>\*\*</sup> More commonly, the reflectivity is defined as the modulus squared of the complex reflection coefficients and therefore corresponds to the ratio of reflected to incident intensity. The reflectivities  $R_s$  and  $R_p$  used throughout this report represent the ratio of reflected to incident amplitude.

$$R_s = \sqrt{\frac{(\cos\phi - A)^2 + B^2}{(\cos\phi + A)^2 + B^2}}$$

$$R_s = \sqrt{\frac{A^2 + B^2 - 2A \cos\phi + \cos^2\phi}{A^2 + B^2 + 2A \cos\phi + \cos^2\phi}} \quad (114)$$

Taking the square of the modulus of Eq. (109)

$$\tan^2\psi = \frac{(A + \sin\phi \tan\phi)^2 + B^2}{(A - \sin\phi \tan\phi)^2 + B^2}$$

$$\tan^2\psi = \frac{A^2 + B^2 + 2A \sin\phi \tan\phi + \sin^2\phi \tan^2\phi}{A^2 + B^2 - 2A \sin\phi \tan\phi + \sin^2\phi \tan^2\phi} \quad (115)$$

But by Eqs. (65) and (67),

$$\tan^2\psi = |\rho|^2 = r_s r_s^* / r_p r_p^*$$

If

$$r_p r_p^* \equiv R_p^2$$

then

$$R_p^2 = \frac{R_s^2}{\tan^2\psi} \quad (116)$$

Thus, substituting from Eq. (115),

$$R_p = R_s \sqrt{\frac{A^2 + B^2 - 2A \sin\phi \tan\phi + \sin^2\phi \tan^2\phi}{A^2 + B^2 + 2A \sin\phi \tan\phi + \sin^2\phi \tan^2\phi}} \quad (116a)$$

F. Summary (Determination of Ellipse Parameters From Optical Constants)

Measured values of  $\psi$  and  $\Delta$  can be predicted for given values of  $n$ ,  $\kappa$  and  $\phi$  as follows. One first finds the intermediate variables  $N$ ,  $A$  and  $B$  from

$$N \equiv n/n_0 \quad (92)$$

$$A^2 = \frac{1}{2} \left[ +\sqrt{[N^2(1-\kappa^2) - \sin^2\phi]^2 + 4N^4\kappa^2} + N^2(1-\kappa^2) - \sin^2\phi \right] \quad (107)$$

$$B^2 = \frac{1}{2} \left[ +\sqrt{[N^2(1-\kappa^2) - \sin^2\phi]^2 + 4N^4\kappa^2} - N^2(1-\kappa^2) + \sin^2\phi \right] \quad (108)$$

Take the positive square root each time to get  $A, B, \geq 0$ . Then  $\Delta$  can be computed for each angle of incidence  $\phi$  from

$$\tan\Delta = -\frac{2B \sin\phi \tan\phi}{(A^2 + B^2) - \sin^2\phi \tan^2\phi} \quad (112)$$

$$-\pi \leq \Delta \leq 0$$

In addition,  $\tan\psi$  can be found from

$$\tan^2\psi = \frac{A^2 + B^2 + 2A \sin\phi \tan\phi + \sin^2\phi \tan^2\phi}{A^2 + B^2 - 2A \sin\phi \tan\phi + \sin^2\phi \tan^2\phi} \quad (115)$$

As discussed earlier,  $\pi/4 \leq \psi \leq \pi/2$ , so the positive square root of Eq. (115) gives  $\tan\psi$ .

If desired, the reflectivities (based on amplitude) may be calculated from

$$R_s \equiv \sqrt{r_s r_s^*} = \sqrt{\frac{A^2 + B^2 - 2A \cos\phi + \cos^2\phi}{A^2 + B^2 + 2A \cos\phi + \cos^2\phi}} \quad (114)$$

$$R_p \equiv \sqrt{r_p r_p^*} = R_s / \tan \psi \quad (116)$$

A FORTRAN program (named MER) which calculates  $\psi$  and  $\Delta$ ,  $R_s$ ,  $R_p$  for metallic reflection from given values of  $n$ ,  $\kappa$  and  $\phi$  is given in Chapter IV, Section B.

The dependence of  $\Delta$ ,  $\psi$ ,  $R_s$  and  $R_p$  on angle of incidence is illustrated in figures 5-8 (a,b,d) for four typical reflecting materials (well or poorly conducting metals and absorbing or transparent dielectrics). Figures 9-16 show the dependence of the same quantities on the optical constants  $n$  and  $\kappa$  of the reflecting surface for fixed angles of incidence ( $2^\circ$ ,  $45^\circ$ ,  $75^\circ$ ).

CHAPTER III

ABSOLUTE PHASE CHANGES UPON REFLECTION FROM ABSORBING MEDIA

A. Introduction

Measurements with the ellipsometer yield the relative difference in phase Δ between the s and p components of the reflected light. The phase change suffered by the two components relative to the respective incident waves, i.e., the "absolute phase changes<sup>3</sup>" can generally not be measured. Therefore, these quantities which are extremely important for the interpretation of thin film interference<sup>15</sup> have to be derived from ellipsometer measurements via the optical constants of the interface.

B. Derivation of Equations

The Fresnel equations in the form given by Eqs. (57) and (58) can be used to determine the phase changes δ<sub>s</sub> and δ<sub>p</sub> that the normal and parallel components of elliptically polarized light undergo upon reflection from absorbing media. As discussed in Chapter II, section A, a positive phase difference δ<sub>s</sub> or δ<sub>p</sub> will be interpreted as being equal to an advance in time while a negative phase difference will mean a retardation.

To simplify the following calculations, these definitions are used.

$$\left. \begin{aligned}
 R_s &\equiv \frac{|E''_s|}{|E_s|} \\
 R_p &\equiv \frac{|E''_p|}{|E_p|}
 \end{aligned} \right\} \quad (93)$$

The E's have their usual meaning illustrated in Fig. 2.

Then, by Eqs. (93), (58), (60a), and (64),

$$r_p = \frac{n_o \cos \phi' - n_c \cos \phi}{n_o \cos \phi' + n_c \cos \phi} = R_p e^{-i\delta_p} \quad (94)$$

By eq. (75)

$$n_c \cos \phi' = a + ib$$

$$r_p = \frac{n_o(a+ib) - n_c^2 \cos \phi}{n_o(a+ib) + n_c^2 \cos \phi} = R_p e^{-i\delta_p} \quad (95)$$

Let

$$A' \equiv n_o a$$

and

$$B' \equiv n_o b$$

Then,

$$r_p = \frac{(A' + iB') - n_c^2 \cos \phi}{A' + iB' + n_c^2 \cos \phi} = R_p e^{-i\delta_p}$$

Expand  $n_c^2$  and write  $e^{-i\delta_p} = \cos \delta_p - i \sin \delta_p$  to get

$$\frac{A' + iB' - n^2(1-\kappa^2)\cos\phi - 2in^2\kappa\cos\phi}{A' + iB' + n^2(1-\kappa^2)\cos\phi + 2in^2\kappa\cos\phi} = R_p (\cos \delta_p - i \sin \delta_p)$$

Multiply both sides by the denominator of the left side and collect real and imaginary parts to obtain

$$A' - n^2(1-\kappa^2)\cos\phi - i(2n^2\kappa\cos\phi - B') =$$

$$R_p \left\{ \left[ A' + n^2(1-\kappa^2)\cos\phi \right] \cos \delta_p + (B' + 2n^2\kappa\cos\phi) \sin \delta_p \right\}$$

$$-iR_p \left\{ \left[ A' + n^2(1-\kappa^2)\cos\phi \right] \sin \delta_p - (B' + 2n^2\kappa\cos\phi) \cos \delta_p \right\}$$

Equate real and imaginary parts of this last equation to get

$$A' - n^2(1-\kappa^2)\cos\phi = R_p \left\{ \left[ A' + n^2(1-\kappa^2)\cos\phi \right] \cos \delta_p + (B' + 2n^2\kappa\cos\phi) \sin \delta_p \right\} \quad (96a)$$



$$B' - 2n^2 \kappa \cos \phi = R_p \left\{ \left[ B' + 2n^2 \kappa \cos \phi \right] \cos \delta_p - \left[ A' + n^2 (1 - \kappa^2) \cos \phi \right] \sin \delta_p \right\} \quad (96b)$$

Equations (96a) and (96b) can be solved for  $\cos \delta_p$  and  $\sin \delta_p$  using determinates. When  $\cos \delta_p$  and  $\sin \delta_p$  are known,  $\tan \delta_p$  can be calculated.

Let the determinant of the coefficients of Eqs. (96a) and (96b) be

$$D_p = R_p \begin{vmatrix} A' + n^2 (1 - \kappa^2) \cos \phi & B' + 2n^2 \kappa \cos \phi \\ B' + 2n^2 \kappa \cos \phi & -[A' + n^2 (1 - \kappa^2) \cos \phi] \end{vmatrix}$$

Then,

$$\cos \delta_p = \frac{1}{D_p} \begin{vmatrix} A' - n^2 (1 - \kappa^2) \cos \phi & R_p (B' + 2n^2 \kappa \cos \phi) \\ B' - 2n^2 \kappa \cos \phi & -R_p (A' + n^2 (1 - \kappa^2) \cos \phi) \end{vmatrix}$$

$$\cos \delta_p = -\frac{R_p}{D_p} \left[ A'^2 - n^4 (1 - \kappa^2)^2 \cos^2 \phi + B'^2 - 4n^4 \kappa^2 \cos^2 \phi \right]$$

$$\cos \delta_p = -\frac{R_p}{D_p} \left\{ A'^2 + B'^2 - n^4 \left[ 4\kappa^2 + \kappa^4 - 2\kappa^2 + 1 \right] \cos^2 \phi \right\}$$

$$\cos \delta_p = -\frac{R_p}{D_p} \left\{ A'^2 + B'^2 - n^4 (1 + \kappa^2)^2 \cos^2 \phi \right\}$$

By Eqs. (81) and (82),  $A' = n_o^2 A$ ,  $B' = n_o^2 B$

$$\cos \delta_p = -\frac{R_p}{D_p} n_o^4 \left\{ A^2 + B^2 - \frac{n^4}{n_o^4} (1 + \kappa^2)^2 \cos^2 \phi \right\} \quad (97)$$

In the same way,

$$\begin{aligned} \sin \delta_p &= \frac{1}{D_p} \begin{vmatrix} R_p (A' + n^2 (1 - \kappa^2) \cos \phi) & A' - n^2 (1 - \kappa^2) \cos \phi \\ R_p (B' + 2n^2 \kappa \cos \phi) & B' - 2n^2 \kappa \cos \phi \end{vmatrix} \\ &= \frac{R_p}{D_p} \left[ A'B' - 2n^2 A' \kappa \cos \phi + B'n^2 (1 - \kappa^2) \cos \phi - 2n^4 \kappa \cos^2 \phi (1 - \kappa^2) \right] \end{aligned}$$

$$\sin \delta_p = -\frac{R_p}{D_p} \frac{-A'B' - 2n_o^2 A' \cos \phi + B'n^2(1-\kappa^2) \cos \phi + 2n_o^4 \kappa \cos^2 \phi (1-\kappa^2)}{2 \cos \phi \left[ 2A'n^2 \kappa - B'n^2(1-\kappa^2) \right]}$$

By eq. (81),

$$A' \equiv n_o a = n_o^2 A$$

By Eq. (82)

$$B' \equiv n_o b = n_o^2 B$$

$$\sin \delta_p = -\frac{R_p}{D_p} 2n_o^2 \cos \phi \left[ 2An^2 \kappa - Bn^2(1-\kappa^2) \right]$$

By Eq. (85)

$$n^2 \kappa = ab = n_o^2 AB$$

By Eq. (84)

$$n^2(1-\kappa^2) = n_o^2(A^2 - B^2 + \sin^2 \phi)$$

Thus,

$$\sin \delta_p = -\frac{R_p}{D_p} 2n_o^4 \cos \phi \left[ 2A^2 B - B(A^2 - B^2 + \sin^2 \phi) \right]$$

$$\sin \delta_p = -\frac{R_p}{D_p} 2n_o^4 B \cos \phi \left[ A^2 + B^2 - \sin^2 \phi \right] \quad (98)$$

Dividing Eq. (98) by Eq. (97),

$$\tan \delta_p = \frac{-\frac{R_p}{D_p} 2n_o^4 B \cos \phi \left[ A^2 + B^2 - \sin^2 \phi \right]}{-\frac{R_p}{D_p} n_o^4 \left\{ A^2 + B^2 - \frac{n_o^4}{4} (1 + \kappa^2)^2 \cos^2 \phi \right\}}$$

$$\tan \delta_p = \frac{2B \cos \phi [A^2 + B^2 - \sin^2 \phi]}{A^2 + B^2 - n_o^4 (1 + \kappa^2)^2 \cos^2 \phi} \quad (99)$$

where

$$N \equiv n/n_o \quad (92)$$

The same procedure can be used to determine  $\tan \delta_s$ . By Eqs. (59a), (64), and (91), Eq. (57) becomes

$$r_s = \frac{n_o \cos \phi - n_c \cos \phi'}{n_o \cos \phi + n_c \cos \phi'} = R_s e^{-i\delta_s} \quad (100)$$

By Eq. (75),

$$n_c \cos \phi' = a + ib$$

$$\frac{n_o \cos \phi - (a + ib)}{n_o \cos \phi + (a + ib)} = R_s e^{-i\delta_s}$$

$$\text{If } a = n_o A \quad (81)$$

$$b = n_o B \quad (82)$$

$$\frac{\cos \phi - A - iB}{\cos \phi + A + iB} = R_s e^{-i\delta_s}$$

$$\frac{(\cos \phi - A) - iB}{(\cos \phi + A) + iB} = R_s (\cos \delta_s - i \sin \delta_s)$$

$$\cos \phi - A - iB = R_s \left\{ \left[ (\cos \phi + A) \cos \delta_s + B \sin \delta_s \right] + i \left[ B \cos \delta_s - (\cos \phi + A) \sin \delta_s \right] \right\}$$

Equate real and imaginary parts to get

$$\cos \phi - A = R_s \left[ (\cos \phi + A) \cos \delta_s + B \sin \delta_s \right] \quad (101a)$$

$$-B = R_s \left[ B \cos \delta_s - (\cos \phi + A) \sin \delta_s \right] \quad (101b)$$

These two equations can be solved by determinants to yield  $\cos \delta_s$  and  $\sin \delta_s$ . If the determinant of the coefficients is  $D_s$ ,

$$D_s \equiv R_s \begin{vmatrix} \cos\phi + A & B \\ B & -(\cos\phi + A) \end{vmatrix}$$

Then,

$$\cos\delta_s = \frac{1}{D_s} \begin{vmatrix} \cos - A & R_s B \\ -B & -R_s(\cos\phi + A) \end{vmatrix}$$

$$\cos\phi_s = \frac{R_s}{D_s} (A^2 - \cos^2\phi + B^2) \quad (102a)$$

$$\sin\phi_s = \frac{1}{D_s} \begin{vmatrix} R_s(\cos\phi + A) & \cos\phi - A \\ R_s B & -B \end{vmatrix}$$

$$\sin\phi_s = \frac{R_s}{D_s} (-B \cos\phi - AB - B \cos\phi + AB)$$

$$\sin\phi_s = -\frac{R_s}{D_s} 2B \cos\phi \quad (102b)$$

Divide Eq. (102b) by Eq. (102a) to get

$$\tan\phi_s = -\frac{2B \cos\phi}{A^2 + B^2 - \cos^2\phi} \quad (103)$$

### C. RANGES OF $\delta_p$ , $\delta_s$

The results of the previous section are equations which give the tangents of the absolute phase changes  $\delta_s$  and  $\delta_p$ . Evaluation of these equations for any given case does not yield  $\delta_s$  and  $\delta_p$  unambiguously on account of the identity

$$\tan(\alpha \pm 180^\circ) = \tan \alpha$$

In this section, a method is presented whereby one can determine  $\delta_s$  and  $\delta_p$

uniquely. Recalling equation (102b) of the previous section:

$$\sin \delta_s = -\frac{R_s}{D_s} 2B \cos \phi \quad (102b)$$

where the positive quantity  $R_s$  was defined as

$$R_s \equiv \left| \frac{E_s''}{E_s} \right| = |r_s|$$

and  $D_s$  is the determinant of the coefficients of (101a) and (101b),

$$\cos \phi - A = R_s [(\cos \phi + A) \cos \delta_s + B \sin \delta_s] \quad (101a)$$

$$-B = R_s [B \cos \delta_s - (\cos \phi + A) \sin \delta_s] \quad (101b)$$

Thus,

$$D_s = \begin{vmatrix} \cos \phi + A & B \\ B & -(\cos \phi + A) \end{vmatrix} = -[(\cos \phi + A)^2 + B^2]$$

Since  $D_s$  is the negative of the sum of two squares,

$$D_s \leq 0.$$

It has been shown that  $b \geq 0$  (see discussion concerning Eq. (75))

and since

$$B \equiv b/n_o, \quad n_o > 0.$$

$B$  is also positive since the angle of incidence  $\phi$  lies on the range

$0 \leq \phi \leq 90^\circ$ ,  $\cos \phi \geq 0$ . With  $R_s > 0$ ,  $B > 0$ ,  $\cos \phi > 0$  and  $D < 0$ , the right-hand side of Eq. (102b) is positive. Therefore,  $\sin \delta_s$  is positive and

$$0 \leq \delta_s \leq \pi.$$

Given that  $\delta_s$  lies in this range and given  $\tan \delta_s$ , it is possible to obtain  $\delta_s$  unambiguously.

It has been shown (Eq. (80)) that the relative phase change  $\Delta$  lies in the range

$$-\pi \leq \Delta \leq 0 \quad (80)$$

Thus, given  $\tan \Delta$  one can determine  $\Delta$  unambiguously. But

$$\Delta \equiv \delta_p - \delta_s \quad (66)$$

so that

$$\delta_p = \Delta + \delta_s \quad (66a)$$

When  $\Delta$  and  $\delta_s$  have been found,  $\delta_p$  is found unambiguously from this equation.

#### D. Summary

The absolute phase changes undergone during reflection by the components polarized normal and parallel to the plane of incidence are given by

$$\tan \delta_s = \frac{-2B \cos \phi}{A^2 + B^2 - \cos^2 \phi} \quad (103)$$

$$\tan \delta_p = \frac{2B \cos \phi [A^2 + B^2 - \sin^2 \phi]}{A^2 + B^2 - N^4 (1 + \kappa^2)^2 \cos^2 \phi} \quad (99)$$

where

$$N \equiv n/n_0 \quad (92)$$

and

$$A = - \frac{\sin\phi \tan\phi \cos 2\phi}{1 - \sin 2\psi \cos\Delta} \quad (81)$$

$$B = - \frac{\sin\phi \tan\phi \sin 2\psi \sin\Delta}{1 - \sin 2\psi \cos\Delta} \quad (82)$$

Again, a positive phase change  $\delta_s$  or  $\delta_p$  is to be interpreted as an advance in time. An advance in time corresponds to a clockwise rotation of the electric vector in the complex plane, since the convention  $e^{-i\omega t}$  has been adopted here to describe the time dependence of the wave. The proper quadrants for  $\delta_s$  and  $\delta_p$  can be found by knowing  $\tan \delta_s$  and  $\tan \Delta$  and by knowing that

$$\begin{aligned} 0 &\leq \delta_s \leq \pi \\ -\pi &\leq \Delta \leq 0 \\ \delta_p &= \Delta + \delta_s \end{aligned}$$

Figures 5-8 (parts c) contain plots showing how the absolute phase changes vary with angle of incidence in four specific cases: a good reflector (Fig. 5), a relatively poor reflector (Fig. 6), a transition material (Fig. 7), and a dielectric (Fig. 8). The dependence of  $\delta_p$  and  $\delta_s$  on the optical constants  $n$  and  $\kappa$  of the reflecting surface is illustrated in Figs. 9, 10, 12, 13, 15, and 16 for fixed angles of incidence of  $2^\circ$ ,  $45^\circ$  and  $75^\circ$ .

## CHAPTER IV

## NUMERICAL RESULTS

Computer programs in FORTRAN - II language have been written for numerical application of the pertinent equations derived in the previous two chapters. For reference purposes, the complete programs are reproduced in this chapter together with typical results and some graphical representations.

A. Optical Constants From Phase Difference and Amplitude Ratio1. Program MOC

The equations necessary for computing the metal optical constants  $n$  and  $\kappa$  from the measured values of  $\phi$ ,  $\psi$  and  $\Delta$  have been derived in Chapter II, Section B. They are

$$A = - \frac{\sin\phi \tan\phi \cos 2\psi}{1 - \sin 2\psi \cos\Delta} \quad (81)$$

$$B = - \frac{\sin 2\psi \sin\phi \tan\phi \sin\Delta}{1 - \sin 2\psi \cos\Delta} \quad (82)$$

$$N^2 = \frac{n^2}{n_o^2} = \frac{1}{2} \left[ + \sqrt{(A^2 - B^2 + \sin^2\phi)^2 + 4A^2B^2} + (A^2 - B^2 + \sin^2\phi) \right] \quad (88a)$$

$$\kappa^2 = \frac{+\sqrt{(A^2 - B^2 + \sin^2\phi)^2 + 4A^2B^2} - (A^2 - B^2 + \sin^2\phi)}{+\sqrt{(A^2 - B^2 + \sin^2\phi)^2 + 4A^2B^2} + (A^2 - B^2 + \sin^2\phi)} \quad (91a)$$

All square roots are positive so that  $N, \kappa \geq 0$ .  $n$  is the real part of the complex refractive index  $n(1+i\kappa)$  of the reflecting medium;  $n_o$  is the refractive index of the transparent incident medium.



The following names of variables are employed in the program MOC

(Metal Optical Constants):

<u>Name</u>	<u>Symbol</u>	<u>Description</u>
PHID	$\phi$ (degrees)	angle of incidence
PHI	$\phi$ (radians)	angle of incidence
DELD	$\Delta$ (degrees)	relative phase change
DEL	$\Delta$ (radians)	relative phase change
PSID	$\psi$ (degrees)	where $\tan\psi =$ relative amplitude attenuation
PSI	$\psi$ (radians)	
A	A	intermediate variable
B	B	intermediate variable
TN	N	$n/n_0$ where $n$ is real part of complex refractive index of metal, and $n_0$ is index of transparent incident medium
TK	$\kappa$	absorption index

Input Cards for Program MOC

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

<u>Card</u>	<u>Col 1</u>	<u>Col 11</u>	<u>Col 21</u>	<u>Col 31</u>	<u>Col 41</u>	<u>Col 51</u>	<u>Col 61</u>
1	Title and comments (up to 80 columns may be used)						
2	$\phi_1$	$\phi_2$	$\phi_3$	$\phi_4$	$\phi_5$	$\phi_6$	$\phi_7$
3	$\Delta_1$	$\Delta_2$	$\Delta_3$	$\Delta_4$	$\Delta_5$	$\Delta_6$	$\Delta_7$
4	$\psi_1$	$\psi_2$	$\psi_3$	$\psi_4$	$\psi_5$	$\psi_6$	$\psi_7$

Card 1 is printed verbatim on the first page of the printout. Cards 2, 3, and 4 constitute a set of input data. Any number of sets may follow this first set. The last set of cards must be followed by a blank card. The data must contain a decimal point and may be located anywhere in the field beginning with the column indicated and ending in the column preceding the next field.

The program together with a sample output is reproduced on the next page.

```

PROGRAM MCC (INPUT,CUTPUT,TAPE2=INPUT,TAPE3=CUTPUT)
C MCC METAL OPTICAL CONSTANTS
DIMENSION PHID(7),PHI(7),DELC(7),DEL(7),PSID(7),A(7),ASQ(7)
C,B(7),BSC(7),TN(7),TNSC(7),TK(7),TKSC(7)
DIMENSION TITLE (E)
1 READ (2,2) TITLE
2 FORMAT (8A1C)
3 WRITE (3,4) TITLE
4 FORMAT (1H1, 8A1C)
1C FORMAT (7F1C,5)
11 FORMAT (7F1C,C)
12 FORMAT(///3X,4PHID,6X,4HCELD,6X,4HPSID,8X,1HA,9X,1PB,9X,2+TN,7X,
C2+TK)
14 FORMAT(1P C//3CX,42H-----METAL OPTICAL CONSTANTS----- )
WRITE(3,14)
25 READ(2,11)(PHID(M),M=1,7)
IF(PHID(1)).EQ.C.0)GC 1C 3C5
READ(2,11)(DELD(M),M=1,7)
READ(2,11)(PSID(M),M=1,7)
DO 1C1 M=1,7
PHI(M)=PHID(M)*C.174533
DEL(M)=DELD(M)*C.174533
PSI(M)=PSID(M)*C.174533
1C1 CONTINUE
DO 2C1 M=1,7
SPH=SIN (PHI(M))
SPHC=SPH*SPH
CPH=CCS (PHI(M))
TPH=SPH/CPH
SD=SIN (DEL(M))
CD=COS (DEL(M))
STPS=SIN (2.C*PSI(M))
CTPS=COS (2.C*PSI(M))
A(M)=-SPH*TPH*CTPS/(1.C-CD*STPS)
B(M)=-SPH*TPH*SD*STPS/(1.0-CD*STPS)
BSC(M)=B(M)*B(M)
E=ASQ(M)-BSC(M)+SPH*SPH
TNSQ(M)=C.5*(SQRT (E+E+4.0*ASQ(M)*BSC(M))+E)
IF (TNSC(M)) 150,152,152
15C TN(M)=C
GO TO 154
152 TN(M)=SQRT (TNSC(M))
154 TKSQ(M)=(SQRT (E+E+4.0*ASQ(M)*BSC(M))-E)/(SQRT (E+E+4.C*ASQ(M)*BSC
C(M))+E)
IF (TKSC(M)) 156,156,158
156 TK(M)=C
GC TC 2C1
158 TK(M)=SQRT (TKSC(M))
2C1 CCNTITLE
WRITE(3,12)
CC 3C1 M=1,7
3C1 WRITE(3,1C)PHID(M),DELD(M),PSID(M),A(M),B(M),TN(M),TK(M)
GO TC 25
2C5 RETLRN
END

```

PROGRAM MCC -- SAMPLE CUTPUT (SILVER)

-----METAL OPTICAL CONSTANTS-----

PHIC	CELD	PSIC	A	B	TA	TK
2.CC000	-C3480	45.CCC9C	.21143	4.CC190	.21144	18.92630
4C.CCCCC	-15.1322C	45.2649C	.15748	4.C5121	.20000	19.99961
45.CCCCC	-15.7C66C	45.46F3C	.15653	4.06186	.19998	20.00154
5C.CCCCC	-25.2162C	45.5866C	.15644	4.C7251	.20000	2C.00028
7C.CCCCC	-64.2C56C	46.2216C	.19471	4.1C864	.20000	2C.CC020
75.CCCCC	-62.3714C	46.24C7C	.19443	4.11471	.20001	15.99548
8C.CCCCC	-107.1275C	46.2658C	.19421	4.11517	.19999	20.00072

## 2. Program AUXCON

Like the program MOC just presented, the FORTRAN II program, AUXCON, calculates the metal optical constants  $n$  and  $\kappa$  from given values of  $\psi$ ,  $\Delta$  and  $\phi$ . In addition, the program finds the auxiliary constants  $n'$ ,  $\kappa'$ ,  $\sigma$ ,  $\epsilon$  and the penetration depth. The equations evaluated by the program are summarized below.

$$A = - \frac{\sin\phi \tan\phi \cos 2\psi}{1 - \sin 2\psi \cos\Delta} \quad (81)$$

$$B = - \frac{\sin\phi \tan\phi \sin 2\psi \sin\Delta}{1 - \sin 2\psi \cos\Delta} \quad (82)$$

$$N^2 \equiv \left(\frac{n}{n_0}\right)^2 = \frac{1}{2} \left[ A^2 - B^2 + \sin^2\phi + \sqrt{(A^2 - B^2 + \sin^2\phi)^2 + 4A^2B^2} \right] \quad (88a)$$

$$\kappa^2 = \frac{\sqrt{(A^2 - B^2 + \sin^2\phi)^2 + 4A^2B^2} - (A^2 - B^2 + \sin^2\phi)}{\sqrt{(A^2 - B^2 + \sin^2\phi)^2 + 4A^2B^2} + (A^2 - B^2 + \sin^2\phi)} \quad (91a)$$

$$\frac{n'}{n_0} = \sin\phi \sqrt{1 + \frac{\tan^2\phi \cos^2 2\psi}{(1 - \sin 2\psi \cos\Delta)^2}} \quad (83a)$$

$$\kappa' = \frac{-\tan\phi \sin 2\psi \sin\Delta}{\sqrt{\tan^2\phi \cos^2 2\psi + (1 - \sin 2\psi \cos\Delta)^2}} \quad (84)$$

$$\sigma = \frac{\omega n \kappa}{2\pi}$$

$$\epsilon = n^2(1 - \kappa^2)$$

$$\text{penetration depth} = \frac{c}{2\omega n' \kappa'}$$

The last three equations are developed in Chapter I, Section C2.

The following names of variables are employed in the program

AUXCON (auxiliary constants):

<u>Name</u>	<u>Symbol</u>	<u>Description</u>
C	c	speed of light in vacuum
PI	$\pi$	ratio of circumference to diameter of circle
WAVEL	$\lambda_0$	vacuum wavelength
OMEGA	$\omega$	angular frequency
PHI	$\phi$ (radians)	angle of incidence
PHID	$\phi$ (degrees)	angle of incidence
DEL	$\Delta$ (radians)	relative phase change (of p with respect to s polarization)
DELD	$\Delta$ (degrees)	relative phase change
PSI	$\psi$ (radians)	arc tangent of relative amplitude attenuation (of s with respect to p polarization)
PSID	$\psi$ (degrees)	arc tangent of relative amplitude attenuation
A	A	intermediate variable
B	B	intermediate variable
TN	$N = n/n_0$	ratio of real part of complex index to index of (transparent) incident medium
TK	..	absorption index
TNP	$n'/n_0$	$n'$ is ratio of phase velocity of light in metal to that in vacuum
TKP	$\kappa'$	auxiliary absorption index
SIGMA	$\sigma$	electrical conductivity
EPSILON	$\epsilon$	dielectric constant
PD		penetration depth

Input Cards for Program AUXCON

The input data for the program AUXCON are punched on cards as illustrated below:

<u>Card</u>	<u>Col 1</u>	<u>Col 11</u>	<u>Col 21</u>
1	Title and comments (up to 80 columns)		
2	$\phi_1$	$\Delta_1$	$\psi_1$
3	$\phi_2$	$\Delta_2$	$\psi_2$
4	$\phi_3$	$\Delta_3$	$\psi_3$
5	$\phi_4$	$\Delta_4$	$\psi_4$

etc.

The first card is a title card and is printed verbatim at the head of the output. The cards that follow give  $\Delta$  and  $\psi$  at various angles of incidence  $\phi$ . There is no limit to the number of data cards that may be used. The last data card must be followed by a blank card.

The program as presented gives valid results only for light of wavelength  $5461\text{\AA}$  (Mercury green line). To analyze data obtained at another wavelength, the statement "WAVEL = 5461.0E-08" must be changed so that the quantity appearing to the right of the equals sign is the wavelength of the incident light. If this wavelength is given in cm (as in the program on the next page), then the penetration depth will also be given in centimeters and the other dimensional constants will be in gaussian units.

The program, together with a sample of output, is reproduced on the next page.

```

FORTRAN II PROGRAM AUXCON(INPLT,OUTPUT,TAPE2=INPUT,TAPE3=OUTPUT)
THIS PROGRAM FINDS THE METAL OPTICAL CONSTANTS N AND KAPPA WHICH
APPEAR IN THE COMPLEX INDEX OF REFRACTION, THE (REAL) RATIO OF
PHASE VELOCITIES N PRIME, THE PARAMETER KAPPA PRIME, THE (REAL)
ELECTRICAL CONDUCTIVITY SIGMA, THE (REAL) DIELECTRIC CONSTANT
EPSILON, AND THE ABSORPTION COEFFICIENT ALPHA AT WAVELENGTH OF
5461 ANGSTROMS.
DIMENSION TITLE (8)
READ (2,5) TITLE
WRITE (3,6) TITLE
WRITE (3,2)
2 FORMAT (//2X, 107H PHI PSI DELTA N N PRIME
C KAPPA KAPPA PRIME SIGMA EPSILON PEN. DEPTH)
3 FORMAT (7F10.5, 2X, 3(E11.4, 2X))
4 FORMAT (2F10.5)
5 FORMAT (E10.1)
6 FORMAT (1H1,///8A10)
C = 2.55776
PI = 3.1415927
WAVEL = 5461.CE-08
CMEGA = 2.C*PI*C/WAVEL
100 CONTINUE
READ (2,4) PHID, DELD, PSID
IF (PHID.EC.C) GO TO 400
110 DEL = CELD*C.C17453
PSI = PSID*C.C17453
PHI = PHID*C.C17453
21 SPH = SIN(PHI)
SPHQ = SPH*SPH
CPH = CCSF(PHI)
TPH = SPH/CPH
SC = SIN(DEL)
CD = CCSF(DEL)
STPS = SIN(2.C*PSI)
CTPS = CCSF(2.C*PSI)
A = -SPH*TPH*CTPS/(1.C - CD*STPS)
ASQ = A*A
B = -SPH*TPH*SD*STPS/(1.C - CD*STPS)
BSQ = B*B
E = ASQ - BSQ + SPH*SPH
TKSQ = C.5*(SQRT(E+E + 4.0*ASC*BSQ) + E)
IF (TKSQ) 150, 152, 152
150 TK = C.C
GO TO 154
152 TK = SQRT(TKSC)
154 TKSQ = (SQRT(E+E + 4.0*ASC*BSQ) - E)/(SQRT(E+E + 4.0*ASQ*BSQ)+E)
IF (TKSQ) 156, 156, 156
156 TK = C.C
GO TO 160
158 TK = SQRT(TKSC)
160 CONTINUE
TMP = SPH*SQRT(1.0 + (TPH**2*CTPS**2)/(1.0 - STPS*CD)**2)
TKP = -TPH*STPS*SC/SQRT(TPH**2*CTPS**2 + (1.0 - STPS*CD)**2)
SIGMA = CMEGA*TK*TK/(2.C*PI)
EPSILCN = TK*TK*(1.C - TK*TK)
PC = C/(2.C*CMEGA*TKP*TKP)
WRITE (3,3) PHID, PSID, DELD, TK, TPH, TK, TKP, SIGMA, EPSILCN, PC
GO TO 100
400 CONTINUE
END

```

PROGRAM AUXCON -- SAMPLE OUTPUT (SILVER)

	PHI	PSI	DELTA	N	N PRIME	KAPPA	KAPPA PRIME	SIGMA	EPSILON	PEN. DEPTH
2.CCCCC	45.00000	-0.34200		.03362	.04846	115.34870	82.80797	7.4054E+C3	-1.6100E+01	1.0830E-06
40.CCCCC	45.36450	-15.12220		.19550	.67231	20.04215	6.02577	4.3822E+C4	-1.5960E+01	1.0727E-06
45.CCCCC	45.46830	-15.76660		.19965	.73392	20.03504	5.53438	4.3837E+C4	-1.5960E+01	1.0659E-06
50.CCCCC	45.58860	-25.21620		.19973	.79076	20.02661	5.15005	4.3855E+C4	-1.5959E+01	1.0671E-06
70.CCCCC	46.22160	-64.20590		.19986	.95962	20.01295	4.28132	4.3882E+C4	-1.5958E+01	1.0578E-06
75.CCCCC	46.34070	-82.37140		.19987	.98527	20.01117	4.17594	4.3984E+C4	-1.5958E+01	1.0562E-06
80.CCCCC	46.28980	-107.13750		.19985	1.00374	20.01302	4.10336	4.3976E+C4	-1.5956E+01	1.0551E-06

## B. Phase Difference and Amplitude Ratio From Optical Constants

### 1. Program MER

The equations necessary for computing the parameters  $\psi$ ,  $\Delta$ ,  $\delta_s$ ,  $\delta_p$ ,  $R_s$  and  $R_p$ , for metallic reflection from given values of  $n$ ,  $\kappa$ , and  $\phi$  have been derived in Section D of Chapter III and Section A of Chapter III. They are summarized below.

$$A^2 = \frac{1}{2} \left[ +\sqrt{[N^2(1-\kappa^2) - \sin^2\phi]^2 + 4N^4\kappa^2} + N^2(1-\kappa^2) - \sin^2\phi \right] \quad (107)$$

$$B^2 = \frac{1}{2} \left[ +\sqrt{[N^2(1-\kappa^2) - \sin^2\phi]^2 + 4N^4\kappa^2} - N^2(1-\kappa^2) + \sin^2\phi \right] \quad (108)$$

(Positive square root gives A and B)

$$R_s = \sqrt{\frac{A^2 + B^2 - 2A \cos\phi + \cos^2\phi}{A^2 + B^2 + 2A \cos\phi + \cos^2\phi}} \quad * \quad (114)$$

$$R_p = R_s \sqrt{\frac{A^2 + B^2 - 2A \sin\phi \tan\phi + \sin^2\phi \tan^2\phi}{A^2 + B^2 + 2A \sin\phi \tan\phi + \sin^2\phi \tan^2\phi}} \quad * \quad (116a)$$

$$\tan \delta_s = -\frac{2B \cos\phi}{A^2 + B^2 - \cos^2\phi} \quad (103)$$

---

\*  $R_s$  and  $R_p$  are the amplitudes of the reflection coefficients.

The ratios of reflected to incident intensity for polarization parallel and normal to the plane of incidence are  $R_p^2$  and  $R_s^2$  respectively.



$$\tan \delta_p = \frac{2B \cos \phi (A^2 + B^2 - \sin^2 \phi)}{A^2 + B^2 - N^4 (1 + \kappa^2)^2 \cos^2 \phi} \quad (99)$$

$$\tan \Delta = - \frac{2B \sin \phi \tan \phi}{A^2 + B^2 - \sin^2 \phi \tan^2 \phi} \quad (112)$$

$$\tan^2 \psi = \frac{A^2 + B^2 + 2A \sin \phi \tan \phi + \sin^2 \phi \tan^2 \phi}{A^2 + B^2 - 2A \sin \phi \tan \phi + \sin^2 \phi \tan^2 \phi} = \frac{R_s^2}{R_p^2} \quad (115)$$

The following names of variables are employed in program MER  
(metallic reflection).

<u>Name</u>	<u>Symbol</u>	<u>Description</u>
TN2, TN	$N = n/n_o$	ratio of real part of complex refractive index of metal to that of incident medium
TK	$\kappa$	absorption index
PHID	$\phi$ (degrees)	angle of incidence
PHI	$\phi$ (radians)	angle of incidence
A	A	intermediate variable
B	B	intermediate variable
RS	$R_s$	modulus of complex reflection coefficient, reflectivity based on amplitude or amplitude attenuation of s polarization
RP	$R_p$	modulus of complex reflection coefficient, reflectivity based on amplitude of amplitude attenuation of p polarization
DELD	$\Delta$ (degrees)	relative phase change $\delta_p - \delta_s$
DEL	$\Delta$ (radians)	relative phase change
TAND	$\tan\Delta$	
DELP	$\delta_p$ (radians)	"absolute" phase change with respect to incident wave (p polarization)
DELPD	$\delta_p$ (degrees)	" "
DELS	$\delta_s$ (radians)	" (s polarization)
DELSD	$\delta_s$ (degrees)	" "
TANDP	$\tan\delta_p$	
TANDS	$\tan\delta_s$	
PSID	$\psi$ (degrees)	arctangent of relative amplitude attenuation
PSI	$\psi$ (radians)	" "
TAPSI	$\tan\psi$	relative amplitude attenuation of s to p polarization

Input Cards for Program MER

The input data for the program MER are punched on cards as illustrated below.

<u>Card</u>	<u>Col 1</u>	<u>Col 11</u>	<u>Col 21</u>	<u>Col 31</u>	<u>Col 41</u>	<u>Col 51</u>	<u>Col 61</u>
1	Title and comments (up to 80 columns may be used)						
2	n	$\kappa$					
3	$\phi_1$	$\phi_2$	$\phi_3$	$\phi_4$	$\phi_5$	$\phi_6$	$\phi_7$

Card 1 is printed verbatim on the first page of the printout. Cards 2 and 3 constitute a set of input data. Any number of sets may follow the first one. The last set of cards must be followed by a blank card.

The program is reproduced on the next page.

2. Tables

Output tables produced by the program MER which give the complex reflection coefficients  $r_s$  and  $r_p$  separated into amplitude attenuation R and phase change  $\delta$  along with the amplitude ratio  $\tan\psi$  and relative phase change  $\Delta$  of s and p component for various n and  $\kappa$  are reproduced in Appendix II.

3. Graphs

A quantitative illustration of the relationships discussed in this report has been attempted by the graphic representation of numerical results given in figures 9-16. Three sets of graphs correspond to incident angles  $2^\circ$ ,  $45^\circ$ , and  $75^\circ$ . Each set contains a plot of amplitude  $R_p$  (or  $R_s$ ) vs absolute phase change  $\delta_p$  (or  $\delta_s$ ) for each n and  $\kappa$ . Included with the  $45^\circ$  and  $75^\circ$  sets are graphs of  $\psi$  vs  $\Delta$  for constant n and  $\kappa$ . No graph of  $\psi$  vs  $\Delta$  is included for  $2^\circ$  incidence since all the data for that case fit on the small rectangle defined by

$$45.00 \leq \psi \leq 45.73$$

$$-0.7185 \leq \Delta \leq -0.0014$$

for the range of  $0.1 \leq n \leq 5$  and  $0.1 \leq \kappa \leq 20$  considered here.

```

PROGRAM MER(INPUT,CUTPLT,TAPE2=INPUT,TAPE3=CUTPUT)
C PER METALLIC REFLECTIC
DIMENSION PHI(7),PHID(7),ASQ(7),A(7),B(7),BSC(7),B(7),RPSC(7),
CRP(7),RSSC(7),RS(7),TAND(7),DELC(7),DELC(7),TANCS(7),CELS(7),
CDELD(7),TANDP(7),DELP(7),CELDP(7),TAPSI(7),PSI(7),PSIC(7)
DIMENSION TITLE (8)
1 FORMAT (E41C)
2 FORMAT (2F1C,C)
3 FORMAT (///)
4 FORMAT (7F1C,C)
5 FORMAT (4EX,4HTN2=,F7.4,10X,3HTK=,F7.4)
6 FORMAT (///5X,4HPHID,7X,1HA,8X,1HB,7X,2HRS,7X,2HRP,6X,5HTANCS,4X,
X5HTANDP,4X,4HTAND,4X,5HTAPSI,4X,5HCELSC,4X,5HDELC,4X,4HDELC, 6X,
X4HPSIC/11F,13F9.4)
7 FORMAT (1P-1)
8 FORMAT (1P-1, ///E41C)
9 READ (2,1) TITLE
WRITE(3,8) TITLE
N = 4
20 READ(2,2)TN2,TK2
N = N + 1
IF (5 - N) 30, 4C, 5C
30 STOP
40 WRITE (3,7)
N = 1
50 CONTINUE
IF (TA2,EC,C,C)GO TC 31C
READ(2,4)(PHID(M),M=1,7)
DO 1CC M=1,7
PHI(M)=PHID(M)*0.0174533
1CC CONTINUE
DO 2CC M=1,7
TN=TN2
TK=TK2
SX=SIN (PHI(M))
CX=CCS (PHI(M))
TX=SX/CX
TEMP1=(TN**2)*(1.C-TX**2)-SX**2
TEMP2=TEMP1**2+4.C*(TA**4)*(TK**2)
ASQ(M)=0.5*(SQRT(TEMP2)+TEMP1)
IF (ASQ(M))110,112,112
110 A(M)=C
GO TC 114
112 A(M)=SQRT (ASQ(M))
114 BSO(M)=C.5*(SQRT(TEMP2)-TEMP1)
IF (BSO(M))116,118,118
116 B(M)=C
GO TC 120
118 B(M)=SQRT (BSO(M))
120 RSSQ(M)=(ASC(M)+BSO(M)-2.0*A(M)*CX+CX*CX)/(ASQ(M)+BSC(M)+2.0*A(M)
C*CX+CX*CX)
IF (RSSQ(M))122,124,124
122 RS(M)=C
GO TC 126
124 RS(M)= SQRT (RSSQ(M))
126 RPSQ(M)=RSSQ(M)*(ASC(M)+BSC(M)-2.0*A(M)*SX+TX+SX*SX*TX*TX)/(ASQ(M)
C+BSC(M)+2.C*A(M)*S*TX+SX*SX*TX*TX)
IF (RPSQ(M))128,130,130
128 RP(M)=C
GO TC 132
130 RP(M)= SQRT (RPSQ(M))

132 TEMP1=2.C*B(M)*CX
TEMP2=ASQ(M)+BSQ(M)-CX*CX
TANDS(M)=-TEMP1/TEMP2
DELS(M) = ATAN(-TEMP1/TEMP2)
DELD(M)=DELS(M)/0.0174533
IF (DELD(M)) 133, 134, 134
133 DELD(M) = DELD(M) * 180.C
134 CONTINUE
TEMP3=2.C*B(M)*CX*(ASC(M)+BSC(M)-SX*SX)
TEMP4=(TA**4.C)*(1.0+TK*TK)**2.0)*CX*CX-(ASC(M)+BSC(M))
TANDP(M)=-TEMP3/TEMP4
TEMP5=2.C*B(M)*SX*TX
TEMP6=ASQ(M)+BSC(M)-SX*SX*TX*TX
TAND(M)=-TEMP5/TEMP6
DEL(M) = ATAN (-TEMP5/TEMP6)
DELD(M)=DEL(M)/0.0174533
IF (DELD(M)) 136, 126, 135
135 DELD(M) = DELD(M) - 180.C
136 CONTINUE
DELPD(M) = DELSD(M) + DELC(M)
TAPSI(M)=RS(M)/RP(M)
PSI(M)=ATAN (TAPSI(M))
PSIC(M)=PSI(M)/0.0174533
2CC CONTINUE
WRITE(3,5)TA2,TK2
WRITE(3,6)(PHID(M),A(M),B(M),RS(M),RP(M),TANCS(M),TANCP(M),TAND(M)
X,TAPSI(M),DELD(M),DELPD(M),DELC(M),PSIC(M),M=1,7)
IF (N - 4) 25C, 30C, 3C
25C WRITE (3,3)
30C GO TC 2C
31C RETURN
END

```

APPENDIX I

Phase Considerations

Interpretation of literature data on the phase change in reflection is often hindered by different sign conventions employed by the authors. The following brief analysis should be helpful to find a common basis for comparison. A graphic representation of the four possible sign combinations for a harmonic oscillator with phase is given in Fig. 4 in the complex plane.

The following algebraic discussion refers to Table III. A wave incident on a reflecting surface may alternately be described by the factors given in line 1 of Table III. If the corresponding reflected waves are given by line 2 the ratio of reflected to incident wave is of the form listed in line 3 with the phase difference  $\delta$  defined as

$$\delta = \theta_2 - \theta_1$$

A comparison of line 3 with the original oscillation without phase (line 4) shows that an increase in  $\delta$  (taken as a positive number) has the same effect as a change in time given in line 5.

Since the time dependence  $e^{-i\omega t}$  has been chosen before in this report and since it is preferable to have a positive  $\delta$  stand for a phase advance, alternate II has been adopted here and forms the basis for all numerical results contained in this report.

Table III Phase Considerations

Alternates	I	II	III	IV
1. Incident wave	$e^{i(\omega t + \theta_1)}$	$e^{-i(\omega t + \theta_1)}$	$e^{i(\omega t - \theta_1)}$	$e^{-i(\omega t - \theta_1)}$
2. Reflected wave	$e^{i(\omega t + \theta_2)}$	$e^{-i(\omega t + \theta_2)}$	$e^{i(\omega t - \theta_2)}$	$e^{-i(\omega t - \theta_2)}$
3. Ratio	$e^{i\delta}$	$e^{-i\delta}$	$e^{-i\delta}$	$e^{i\delta}$
4. Oscillation without phase	$e^{i\omega t}$	$e^{-i\omega t}$	$e^{i\omega t}$	$e^{-i\omega t}$
5. Effect of increase in pos. $\delta$ same as	advance	advance	delay in time	delay
6. Pos. $\delta$ corresponds to	advance	advance	retardation in time	retardation
7. Neg. $\delta$ corresponds to	retardation	retardation	advance in phase	advance

## APPENDIX II

Numerical Results: Reflection Coefficients, Amplitude Ratio, and  
Relative Phase Change for Reflection From Bare Metals

For reference purposes selected output data from the program MER are recorded on the following pages. The variables which appear in the output are

<u>Name</u>	<u>Symbol</u>	<u>Description</u>
TN2	$N = n/n_0$	ratio of real part of complex refractive index to that of incident medium
TK	$\kappa$	absorption index defined in Eq. (14)
PHID	$\phi$	angle of incidence (deg.)
A, B	A, B	intermediate variables
RS, RP	$R_s, R_p$	amplitude reflectivity for s and p polarization
TANDS, TANDP	$\tan \delta_s, \tan \delta_p$	defined by $\delta_p$ and $\delta_s$ below
TAND	$\tan \Delta$	defined by $\Delta$ below
TAPSI	$\tan \psi \equiv R_s/R_p$	amplitude ratio of reflected s and p polarization for unit amplitude incidence
DELS, DELPD	$\delta_s, \delta_p$	phase of reflected s or p polarization with respect to incident waves
DELD	$\Delta = \delta_p - \delta_s$	phase difference between reflected s and p polarization for in-phase incidence
PSID	$\psi$	defined by $\tan \psi$ above

For details, refer to program description in Chapter IV, Section B1.













TE- .0000										TE- .0000										TE- .0000										TE- .0000										TE- .0000									
PP	AA	BB	CC	DD	EE	FF	GG	HH	II	PP	AA	BB	CC	DD	EE	FF	GG	HH	II	PP	AA	BB	CC	DD	EE	FF	GG	HH	II	PP	AA	BB	CC	DD	EE	FF	GG	HH	II	PP	AA	BB	CC	DD	EE	FF	GG	HH	II
1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...













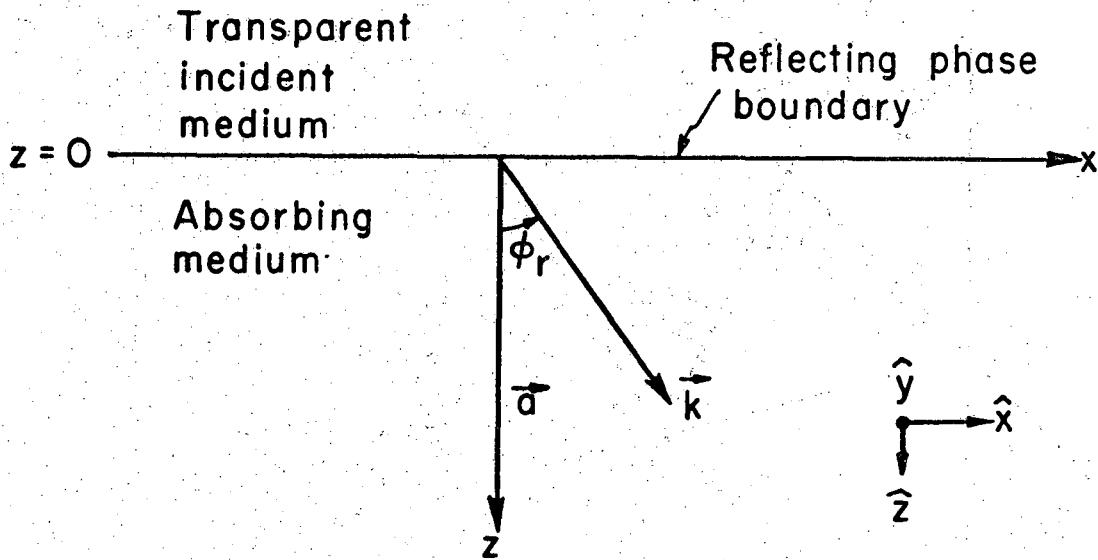


TRZ= 9.0000 TE= 9.0000  
PFC A B  
2.0000 3.0000 30.0000  
40.0000 4.0000 30.0000  
50.0000 4.0000 30.0000  
60.0000 4.0000 30.0000  
70.0000 4.0000 30.0000  
80.0000 4.0000 30.0000  
FANC TAPSI TELCO DELPO DELO PSID  
-0001 1.0000 174.2870 174.2824 -0049 45.0004  
-0390 1.0000 174.2870 174.2824 -0049 45.0004  
-0390 1.0000 174.2870 174.2824 -0049 45.0004  
-0390 1.0000 174.2870 174.2824 -0049 45.0004  
-0390 1.0000 174.2870 174.2824 -0049 45.0004  
-0390 1.0000 174.2870 174.2824 -0049 45.0004  
-0390 1.0000 174.2870 174.2824 -0049 45.0004  
-0390 1.0000 174.2870 174.2824 -0049 45.0004  
-0390 1.0000 174.2870 174.2824 -0049 45.0004

TRZ= 9.0000 TE=10.0000  
PFC A B  
2.0000 3.0000 30.0000  
40.0000 4.0000 30.0000  
50.0000 4.0000 30.0000  
60.0000 4.0000 30.0000  
70.0000 4.0000 30.0000  
80.0000 4.0000 30.0000  
FANC TAPSI TELCO DELPO DELO PSID  
-0001 1.0000 174.2870 174.2824 -0049 45.0004  
-0390 1.0000 174.2870 174.2824 -0049 45.0004  
-0390 1.0000 174.2870 174.2824 -0049 45.0004  
-0390 1.0000 174.2870 174.2824 -0049 45.0004  
-0390 1.0000 174.2870 174.2824 -0049 45.0004  
-0390 1.0000 174.2870 174.2824 -0049 45.0004  
-0390 1.0000 174.2870 174.2824 -0049 45.0004  
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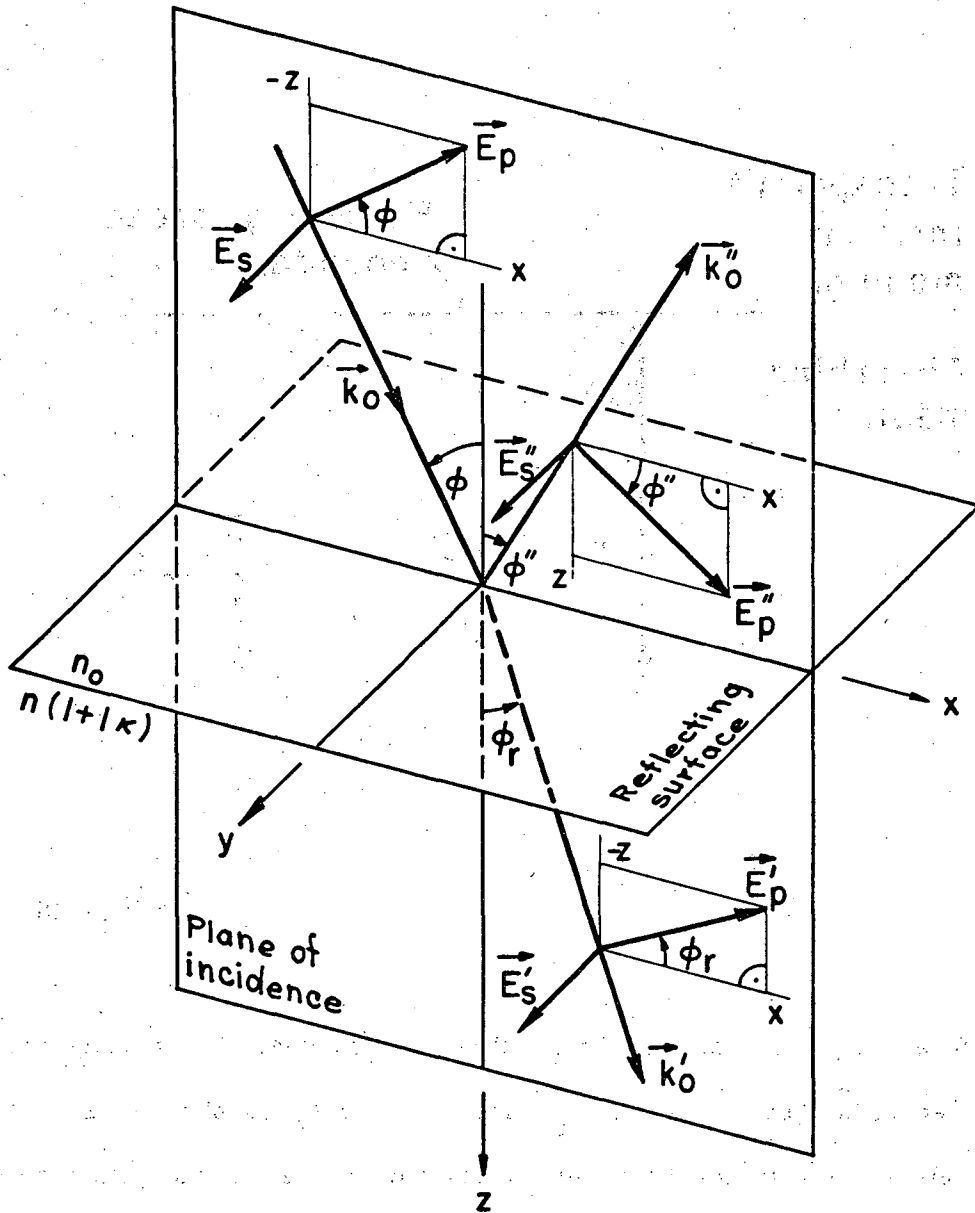
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PFC A B  
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40.0000 4.0000 30.0000  
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70.0000 4.0000 30.0000  
80.0000 4.0000 30.0000  
FANC TAPSI TELCO DELPO DELO PSID  
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-0390 1.0000 174.2870 174.2824 -0049 45.0004

MUB-12609



MUB 12898

Fig. 1 When light propagates in an absorbing medium, the propagation vector  $\vec{k}$  forms an angle  $\phi_r$  with the normal to the surface of the medium while the attenuation vector  $\vec{a}$  lies along the normal. Planes of equal phase are normal to  $\vec{k}$  while planes of equal amplitude are normal to  $\vec{a}$ . The angle  $\phi_r$  is the real angle of refraction in the medium while the plane  $z = 0$  is its surface.



MUB 12905

Fig. 2 Sign conventions for the electric field (positive direction of  $\vec{E}_s$  and  $\vec{E}_p$  in incident, reflected and refracted waves indicated by  $\vec{E}_p$  arrows). The complex index of refraction of the absorbing medium is designated  $n(1 + i\kappa)$ . The subscript p stands for polarization parallel and the subscript s for polarization normal to the plane of incidence.

MUB 12907

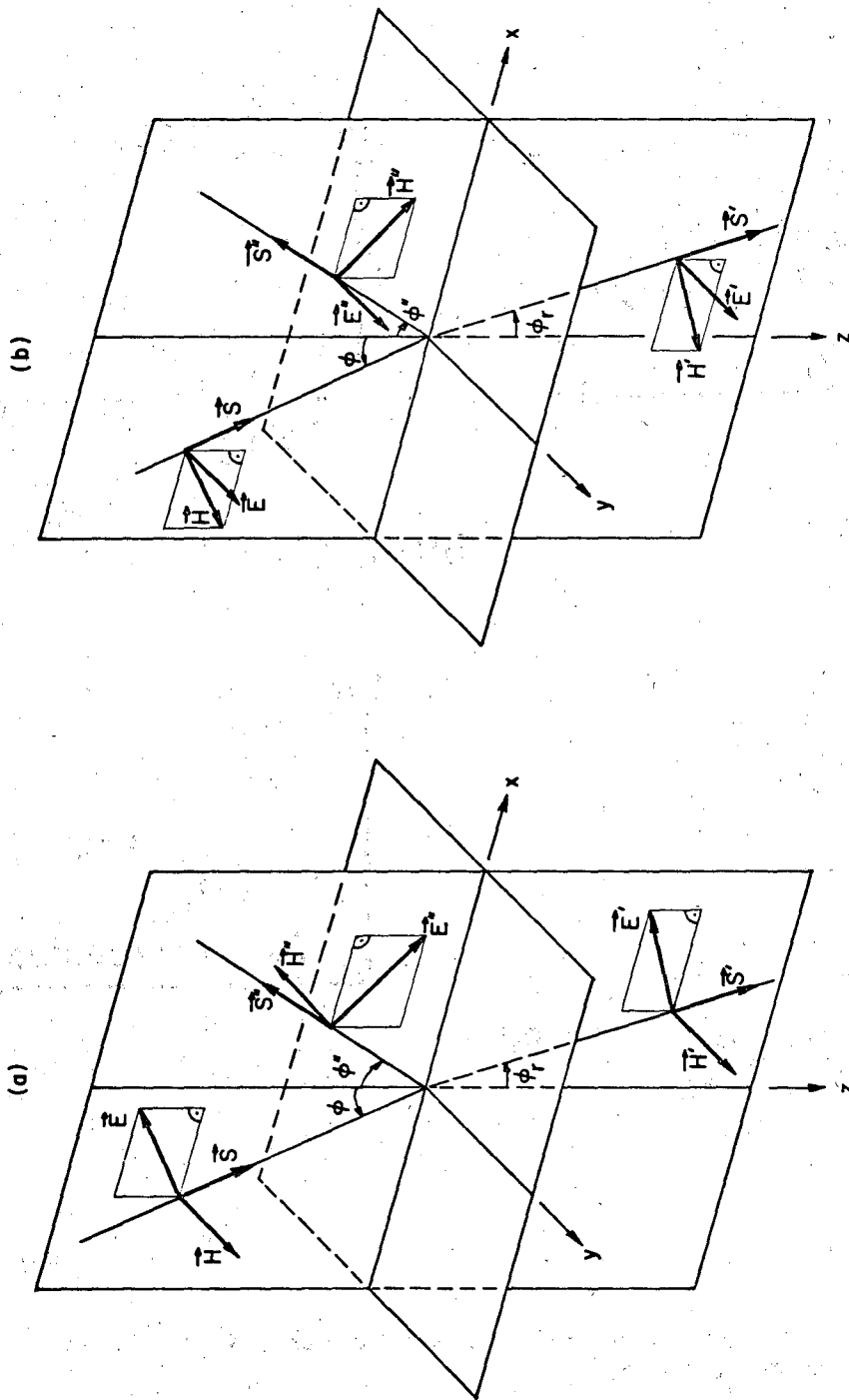
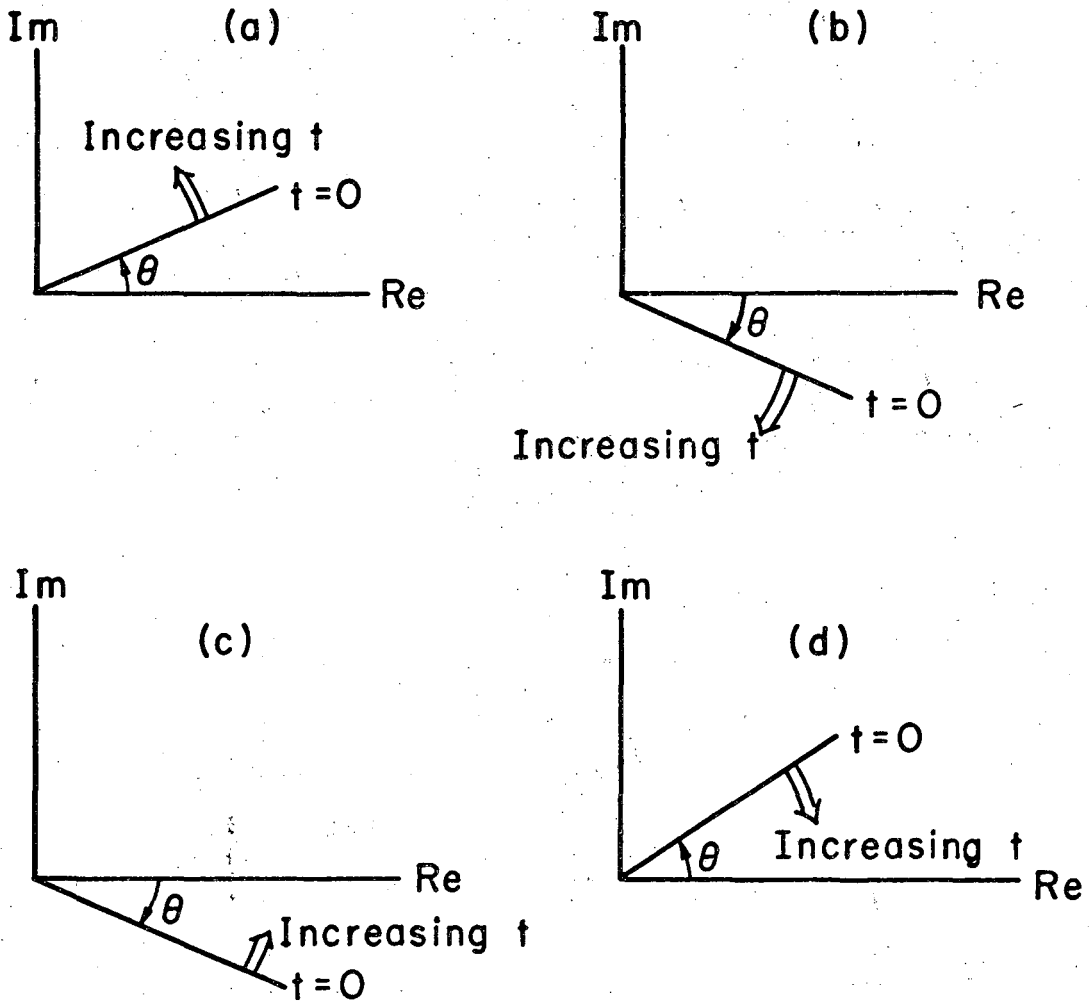


Fig. 3 Reflection and refraction of electromagnetic waves, electric and magnetic fields indicated. (a) Electric vector parallel to plane of incidence. (b) Electric vector normal to plane of incidence.





MUB 12899

Fig. 4 Alternate representations of a harmonic oscillation in the complex plane.  
 (a) alternate I,  $e^{i(\omega t + \theta)}$       (c) alternate III,  $e^{i(\omega t - \theta)}$   
 (b) alternate II,  $e^{-i(\omega t + \theta)}$       (d) alternate IV,  $e^{-i(\omega t - \theta)}$   
 Alternate II has been chosen in this treatment.

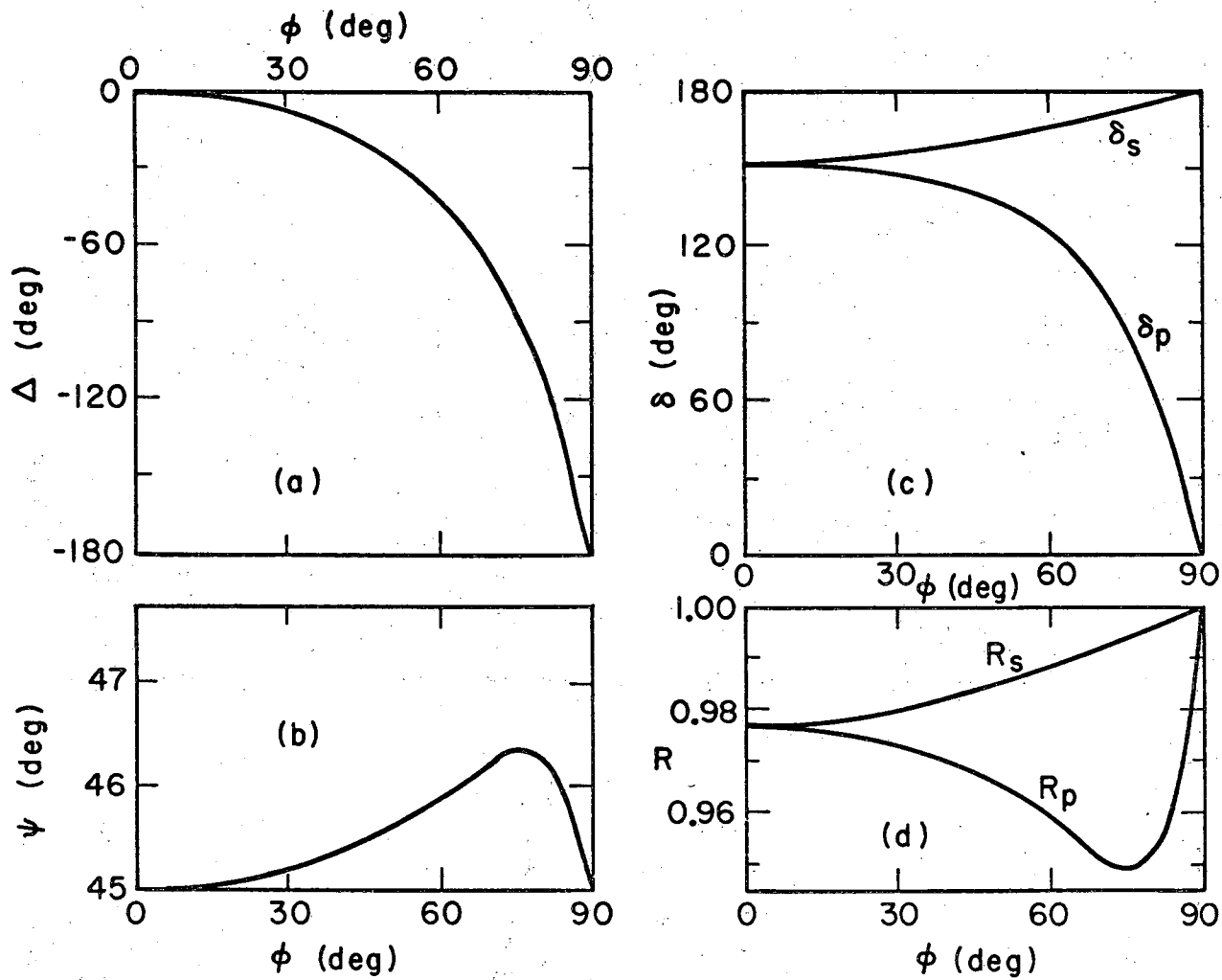


Fig. 5 Relative phase change  $\Delta$ , relative amplitude change  $\psi$ , absolute phase change  $\delta$ , and modulus of reflection coefficient  $R$  as functions of angle of incidence  $\phi$  for a good reflector (silver),  $n = 0.2$ ,  $\kappa = 20$ .

MUB-12913

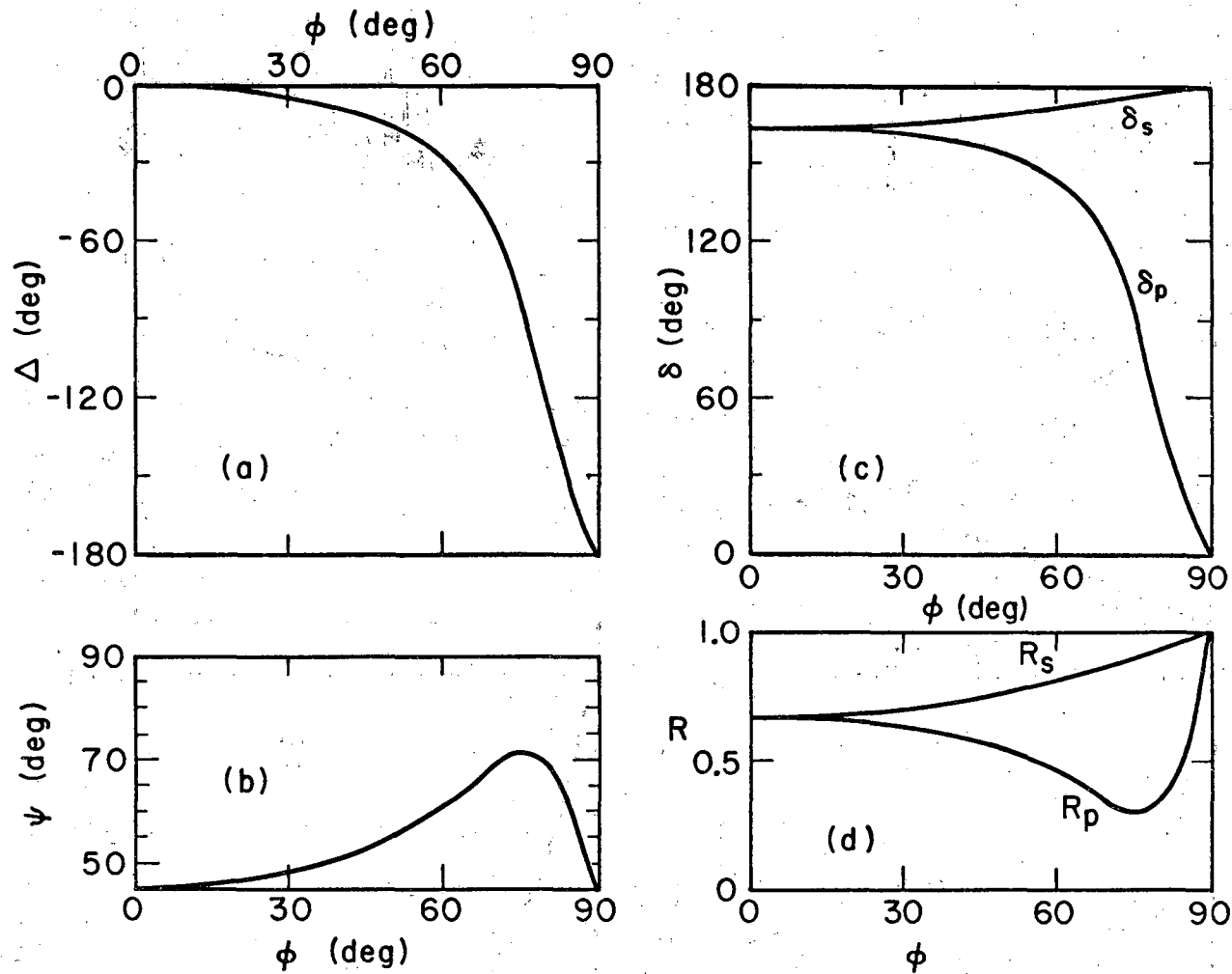


Fig. 6 Relative phase change  $\Delta$ , relative amplitude change  $\psi$ , absolute phase change  $\delta$ , and modulus of reflection coefficient  $R$  as functions of angle of incidence  $\phi$  for a poor reflector (tantalum),  $n = 3.3$ ,  $\kappa = 0.7$ .

MUB-12912

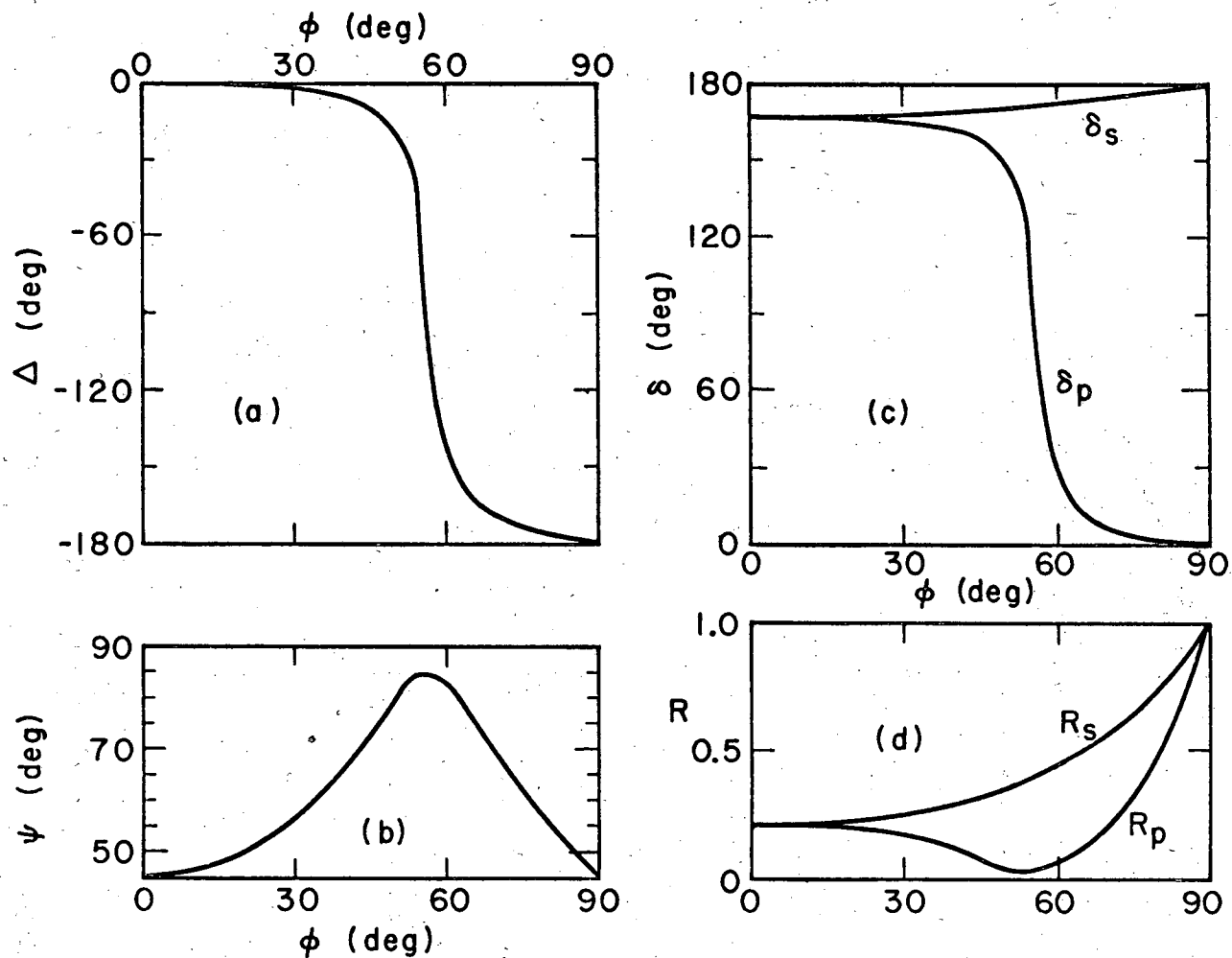


Fig. 7 Relative phase change  $\Delta$ , relative amplitude change  $\psi$ , absolute phase change  $\delta$ , and modulus of reflection coefficient  $R$  as functions of angle of incidence  $\phi$ . Transition between absorbing and dielectric material ("smoked glass")  $n = 1.5$ ,  $\kappa = 0.1$ .

MUB 12911

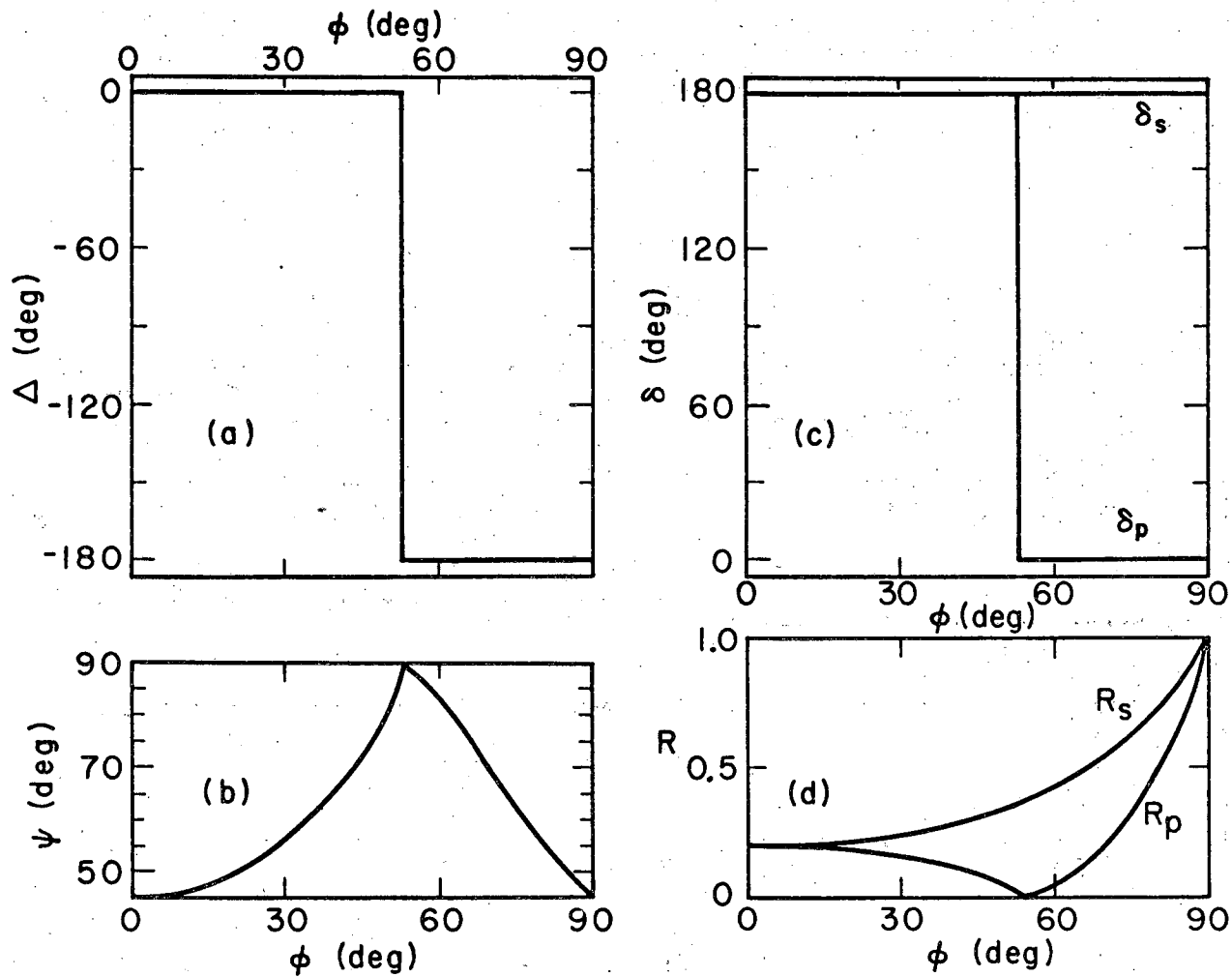
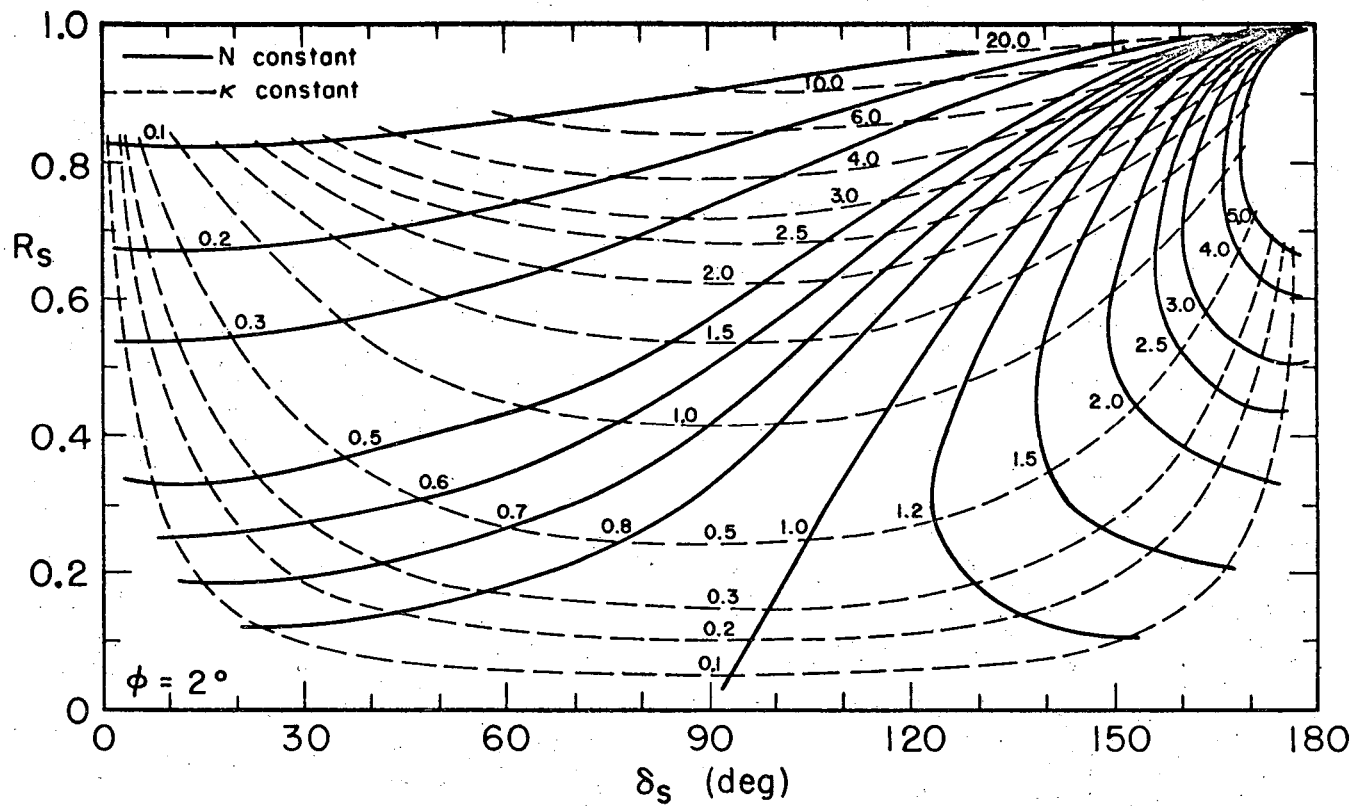


Fig. 8 Relative phase change  $\Delta$ , relative amplitude change  $\psi$ , absolute phase change  $\delta$ , and modulus of reflection coefficient  $R$  as functions of angle of incidence  $\phi$  for a transparent dielectric (glass)  $n = 1.5$ ,  $\kappa = 0$ .

MUB 12906



MUB 12900

Fig. 9 Absolute phase change  $\delta_s$  upon reflection vs. reflected amplitude  $R_s$ , with the optical constants  $n$  and  $\kappa$  of the reflecting material as parameters.  $2^\circ$  angle of incidence; solid lines: constant  $N = n/n_0$ ; broken lines: constant  $\kappa$ .

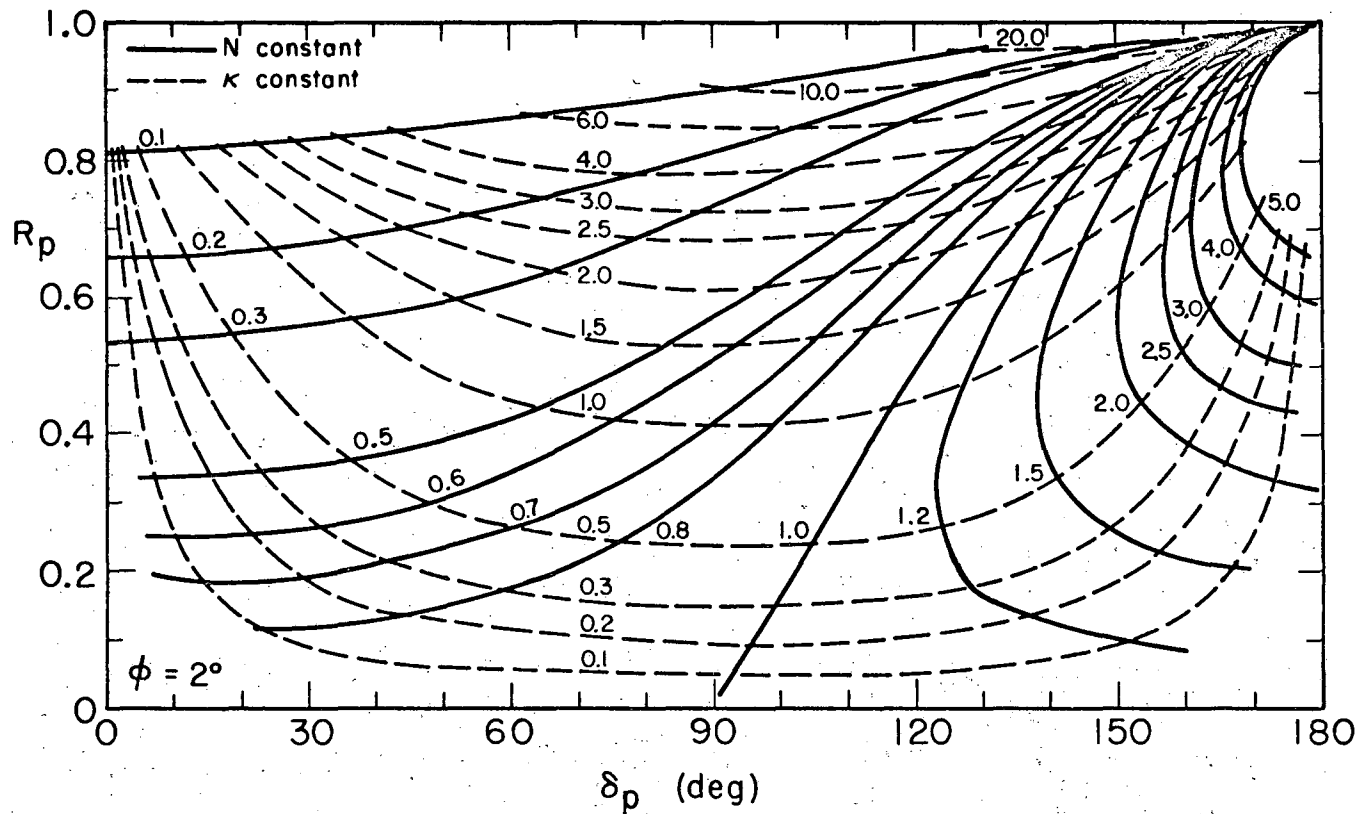


Fig. 10 Absolute phase change  $\delta_p$  upon reflection vs. reflected amplitude  $R_p$ , with the optical constants  $n$  and  $\kappa$  of the reflecting material as parameters.  $2^\circ$  angle of incidence; solid lines: constant  $N = n/n_0$ ; broken lines: constant  $\kappa$ .

MUB 12901

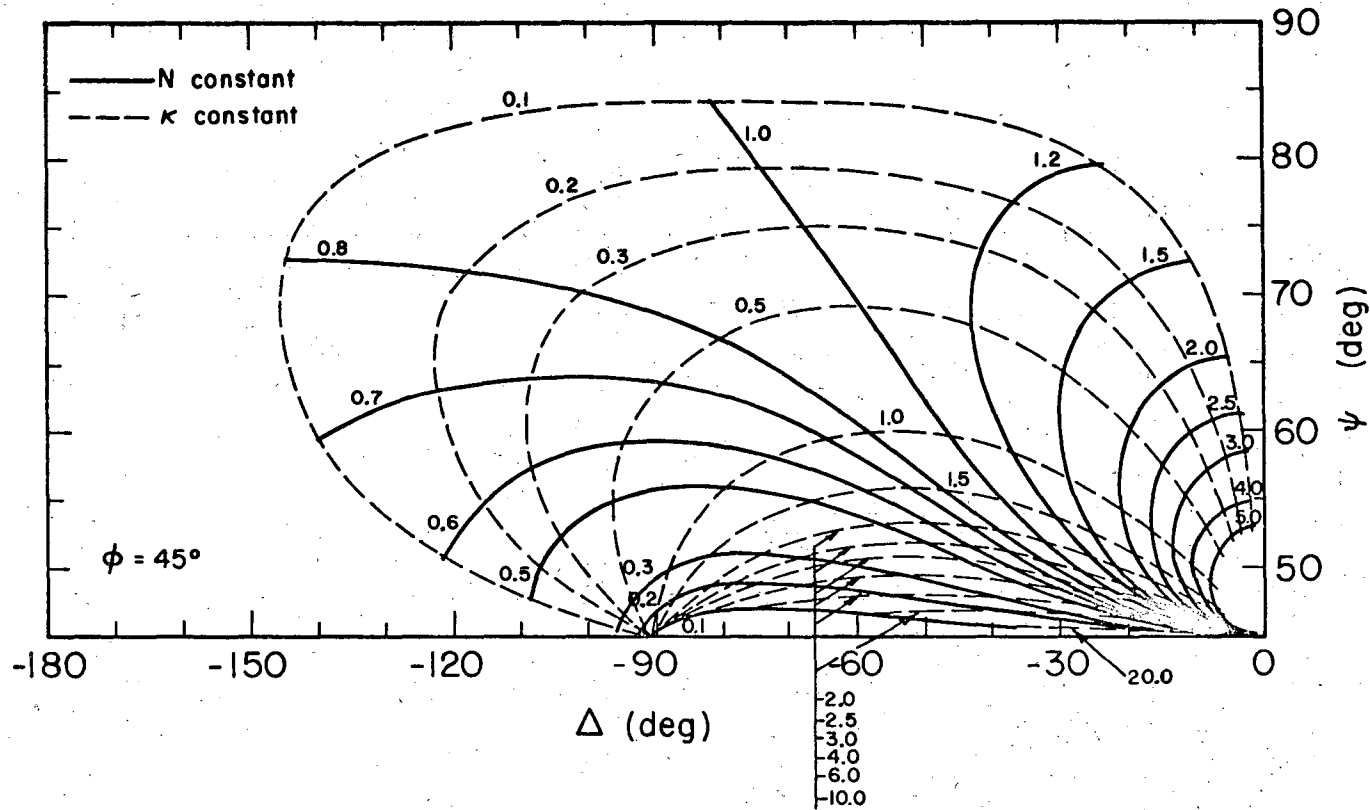
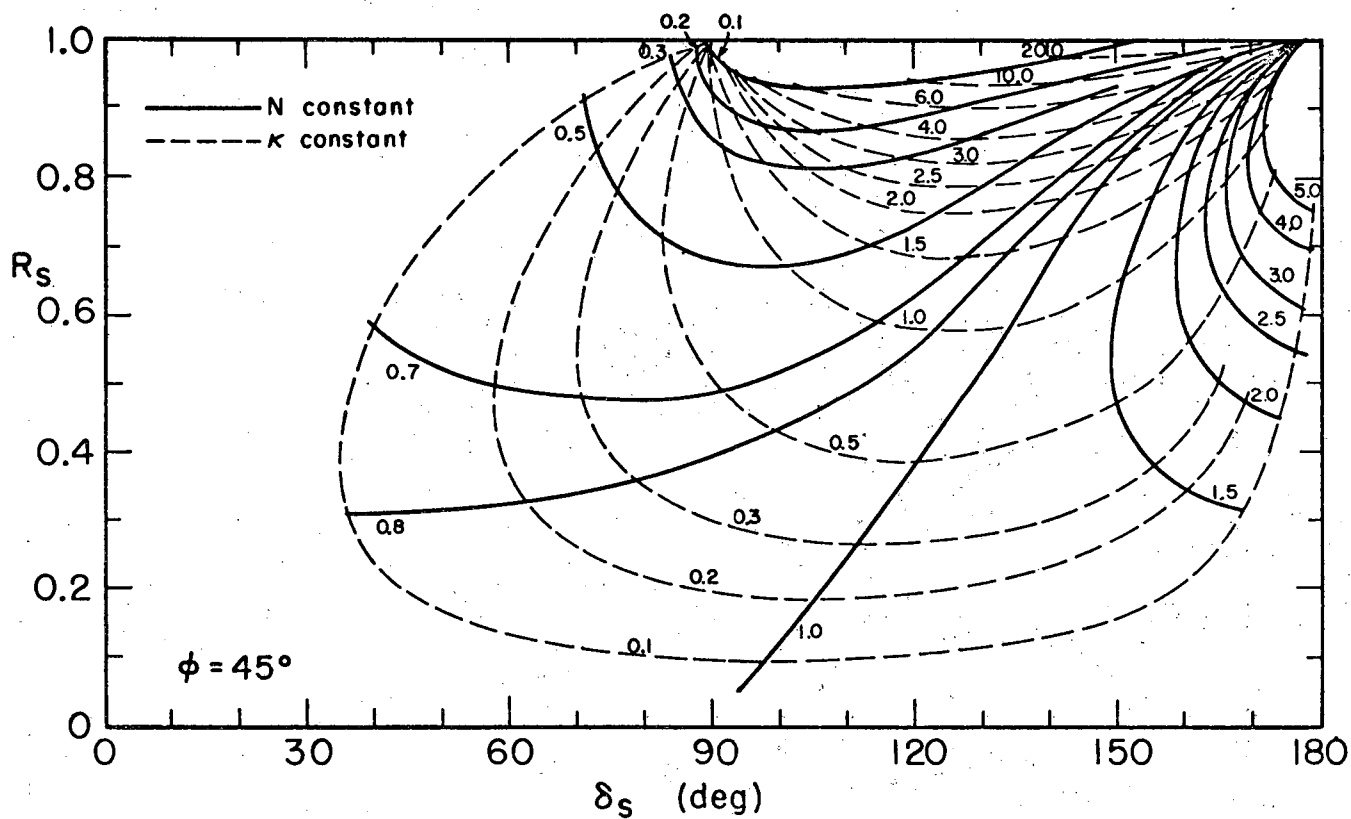


Fig. 11 Relative phase change  $\Delta$  and amplitude change  $\psi$  between s and p polarization with the optical constants  $n$  and  $\kappa$  of the reflecting material as parameters.  $45^\circ$  angle of incidence.

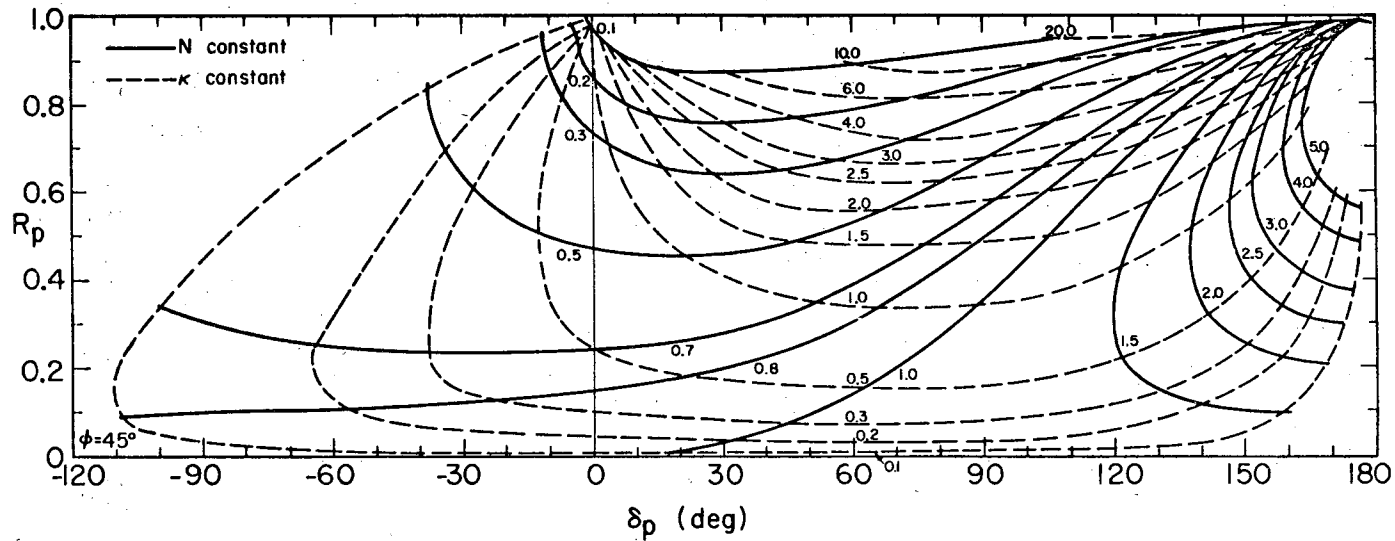
MUB 12902





MUB-12904

Fig. 12 Absolute phase change  $\delta_s$  upon reflection vs. reflected amplitude  $R_s$ , with the optical constants  $n$  and  $\kappa$  of the reflecting material as parameters.  $45^\circ$  angle of incidence; solid lines: constant  $N = n/n_0$ ; broken lines: constant  $\kappa$ .



MUB 12909

Fig. 13 Absolute phase change  $\delta_p$  upon reflection vs. reflected amplitude  $R_p$ , with the optical constants  $n$  and  $\kappa$  of the reflecting material as parameters.  $45^\circ$  angle of incidence; solid lines: constant  $N = n/n_0$ ; broken lines: constant  $\kappa$ .

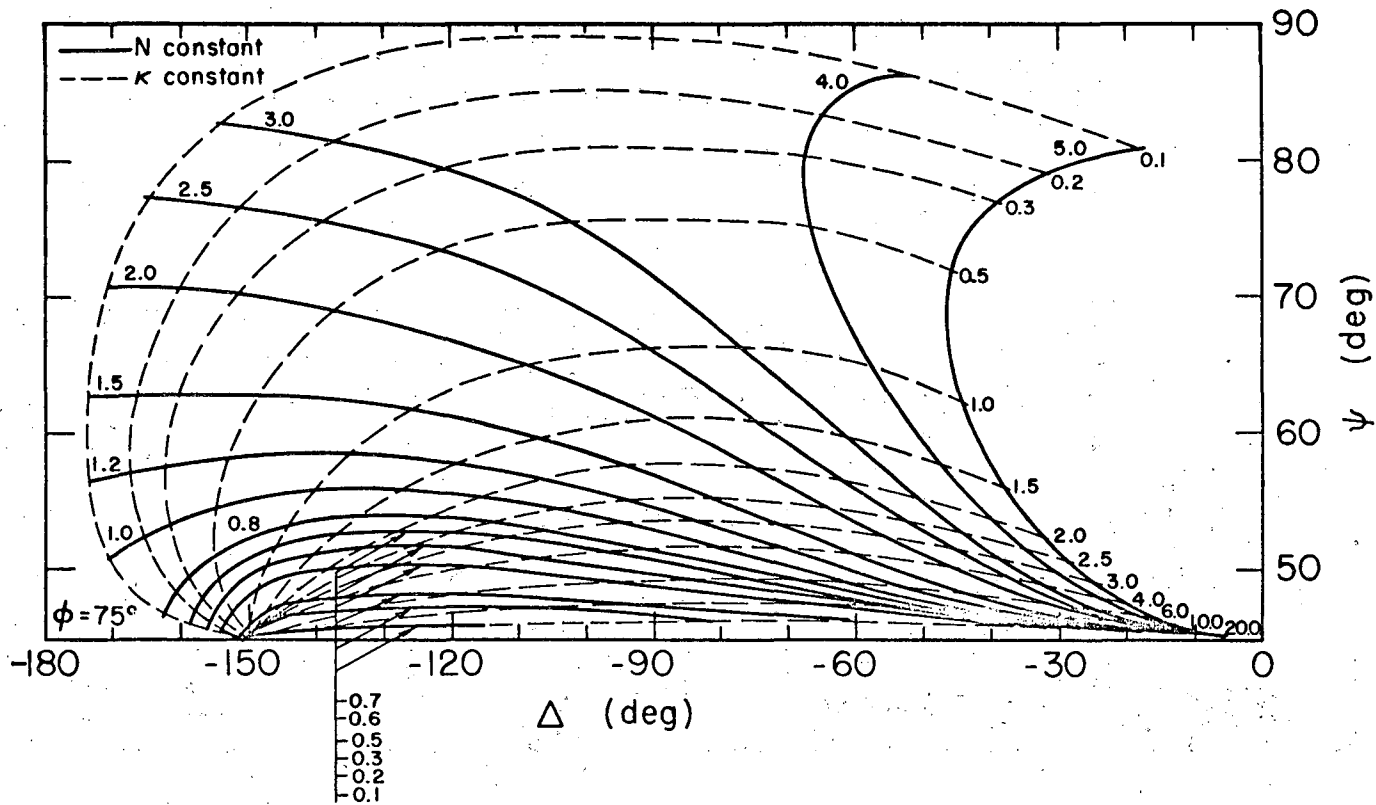


Fig. 14 Relative phase change  $\Delta$  and amplitude change  $\psi$  between s and p polarization with the optical constants  $n$  and  $\kappa$  of the reflecting material as parameters.  $75^\circ$  angle of incidence.

MUB 12910

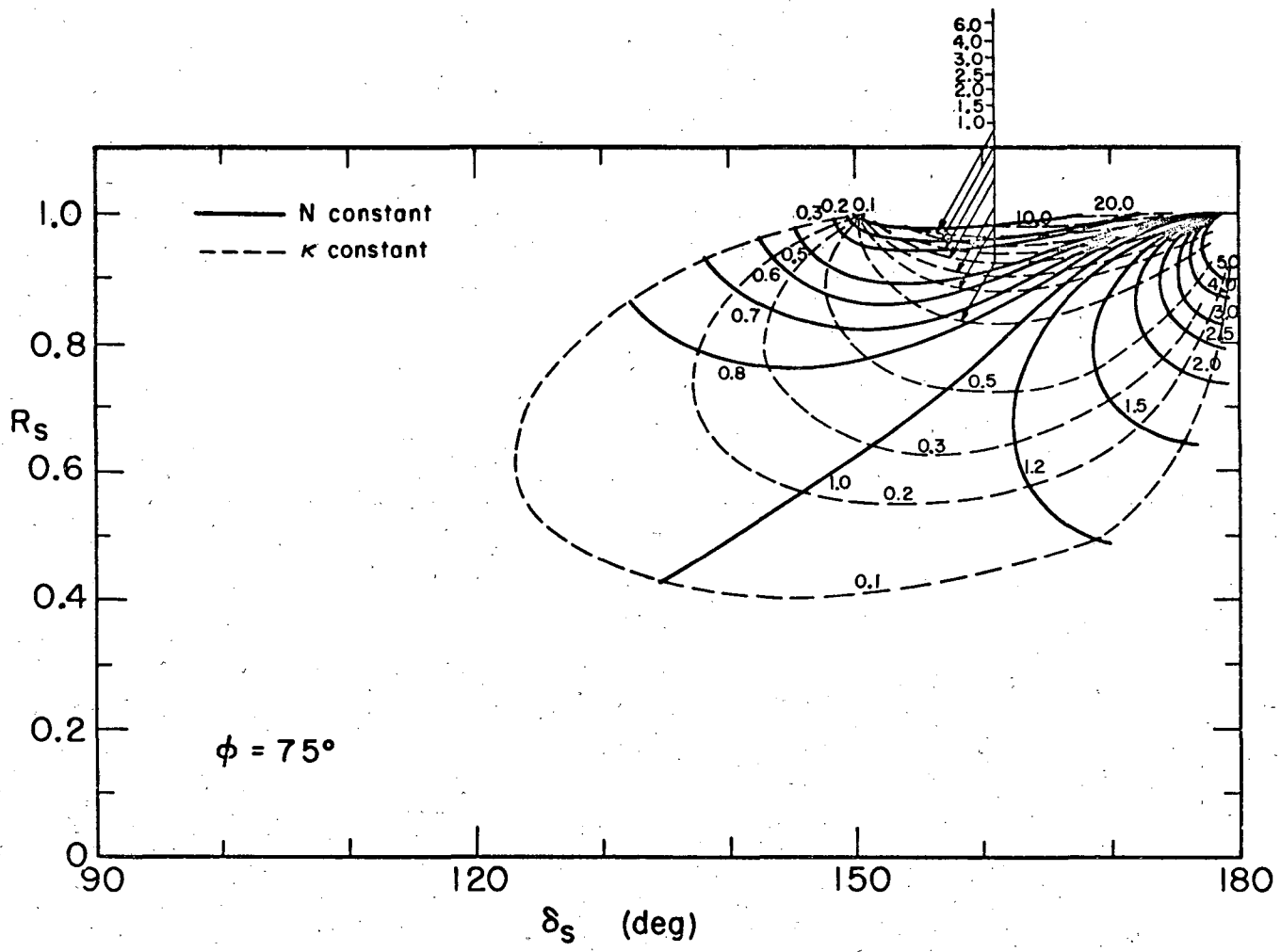
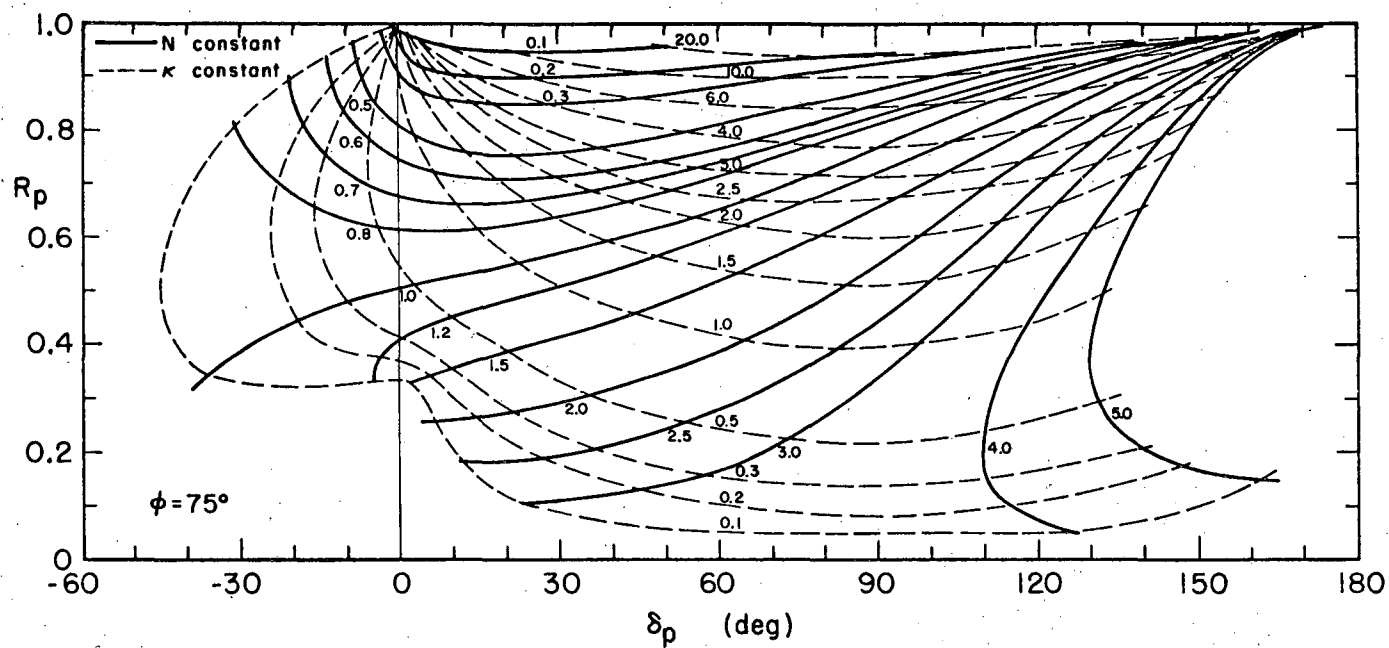


Fig. 15 Absolute phase change  $\delta_s$  upon reflection vs. reflected amplitude  $R_s$ , with the optical constants  $n$  and  $\kappa$  of the reflecting material as parameters.  $75^\circ$  angle of incidence; solid lines: constant  $N = n/n_0$ ; broken lines: constant  $\kappa$ .

MUB-12903



MUB 12908

Fig. 16 Absolute phase change  $\delta_p$  upon reflection vs. reflected amplitude  $R_p$ , with the optical constants  $n$  and  $\kappa$  of the reflecting material as parameters.  $75^\circ$  angle of incidence; solid lines: constant  $N = n/n_0$ ; broken lines: constant  $\kappa$ .

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