12-15-1989

Contours of constant pseudo-Brewster angle in the complex ϵ plane and an analytical method for the determination of optical constants

R. M.A. Azzam
University of New Orleans, razzam@uno.edu

Ericson E. Ugbo

Recommended Citation

R. M. A. Azzam and Ericson E. Ugbo, "Contours of constant pseudo-Brewster angle in the complex ϵ plane and an analytical method for the determination of optical constants," Appl. Opt. 28, 5222-5228 (1989)

Contours of constant pseudo-Brewster angle in the complex ϵ plane and an analytical method for the determination of optical constants

R. M. A. Azzam and Ericson E. Ugbo

The locus of all points in the complex plane of the dielectric function $\epsilon[\epsilon_r + j\epsilon_i = |\epsilon| \exp(j\theta)]$, that represent all possible interfaces characterized by the same pseudo-Brewster angle ϕ_{pB} of minimum p reflectance, is derived in the polar form: $|\epsilon| = l \cos(\zeta/3)$, where $l = 2(\tan^2\phi_{pB})k$, $\zeta = \arccos(-\cos\theta \cos^2\phi_{pB}/k^3)$, and $k = (1 - ⅔ \sin^2\phi_{pB})^{1/2}$. Families of iso-$\phi_{pB}$ contours for (I) $0° \leq \phi_{pB} \leq 45°$ and (II) $45° \leq \phi_{pB} \leq 75°$ are presented. In range I, an iso-ϕ_{pB} contour resembles a cardioid. In range II, the contour gradually transforms toward a circle centered on the origin as ϕ_{pB} increases. However, the deviation from a circle is still substantial. Only near grazing incidence ($\phi_{pB} > 80°$) is the iso-ϕ_{pB} contour accurately approximated as a circle. We find that $|\epsilon| < 1$ for $\phi_{pB} < 37.23°$, and $|\epsilon| > 1$ for $\phi_{pB} > 45°$. The optical constants n,k (where $n + jk = \epsilon^{1/2}$ is the complex refractive index) are determined from the normal incidence reflectance R_0 and ϕ_{pB} graphically and analytically. Nomograms that consist of iso-R_0 and iso-ϕ_{pB} families of contours in the nk plane are presented. Equations that permit the reader to produce his own version of the same nomogram are also given. Valid multiple solutions (n,k) for a given measurement set (R_o,ϕ_{pB}) are possible in the domain of fractional optical constants. An analytical solution of the $(R_o,\phi_{pB}) \rightarrow (n,k)$ inversion problem is developed that involves an exact (noniterative) solution of a quartic equation in $|\epsilon|$. Finally, a graphic representation is developed for the determination of complex ϵ from two pseudo-Brewster angles measured in two different media of incidence.

I. Introduction

The complex amplitude Fresnel reflection coefficient of a p-polarized monochromatic plane wave of light at the planar interface between two (homogeneous, isotropic, linear, and nonmagnetic) media is given by[1]

$$r_p = \frac{\epsilon \cos\phi - (\epsilon - \sin^2\phi)^{1/2}}{\epsilon \cos\phi + (\epsilon - \sin^2\phi)^{1/2}}, \tag{1}$$

where ϕ is the angle of incidence,

$$\epsilon = \epsilon_1/\epsilon_0, \tag{2}$$

and ϵ_0 (real), ϵ_1 (complex) are the dielectric functions (or constants at a given wavelength) of the media of incidence and refraction, respectively. For a given ϵ, $|r_p|$ is a function of ϕ that reaches a minimum at the so-called pseudo-Brewster angle ϕ_{pB}. When the medium of refraction is also transparent, ϵ is real, and ϕ_{pB} reverts to the exact Brewster angle,

$$\phi_B = \tan^{-1}(\epsilon^{1/2}), \tag{3}$$

at which $|r_p|_{\min} = 0$.

R. M. A. Azzam is with University of New Orleans, Department of Electrical Engineering, Lakefront, New Orleans, Louisiana 70148. When this work was done E. E. Ugbo was with Southern University, Technology Department, New Orleans, Louisiana 70126; he is now with Rockford Engineering Services, P.O. Box 543, Sunol, California 94586.

Received 3 May 1989.
0003-6935/89/245222-07$02.00/0.

The relationship between ϕ_{pB} and complex $\epsilon = \epsilon_r + j\epsilon_i$, or the complex refractive index,

$$N = \epsilon^{1/2} = n + jk, \tag{4}$$

was derived by Humphreys-Owen[2] and by others.[3,4] Following the notation of Ref. 3, ϕ_{pB} is determined, for a given complex ϵ, by solving the cubic equation:

$$(2\epsilon_r + 2|\epsilon|^2)u^3 + (|\epsilon|^4 - 3|\epsilon|^2)u^2 - 2|\epsilon|^4 u + |\epsilon|^4 = 0, \tag{5}$$

where

$$u = \sin^2\phi_{pB}. \tag{6}$$

In this paper we consider the nature of the contours of constant ϕ_{pB} in the complex ϵ (and N) plane both analytically and graphically. Previously, Holl[5] presented a family of constant-ϕ_{pB} contours in the nk plane but without giving any accompanying formula that would permit others to create fresh and accurate sets of those contours.

A second objective of this paper is to further develop a previously suggested method[6] for the determination of n and k from measurements of ϕ_{pB} and the normal incidence reflectance R_o. This is accomplished graphically by providing nomograms of lines of constant ϕ_{pB} and lines of constant R_o in the nk plane, and analytically, by deriving a new and explicit mathematical solution. The analytical solution is an efficient and direct alternative to the numerical iterative scheme of Ref. 6.

Finally, a graphic construction is presented with which complex ϵ of an absorbing medium is determined from two pseudo-Brewster angles measured in two different incidence media.

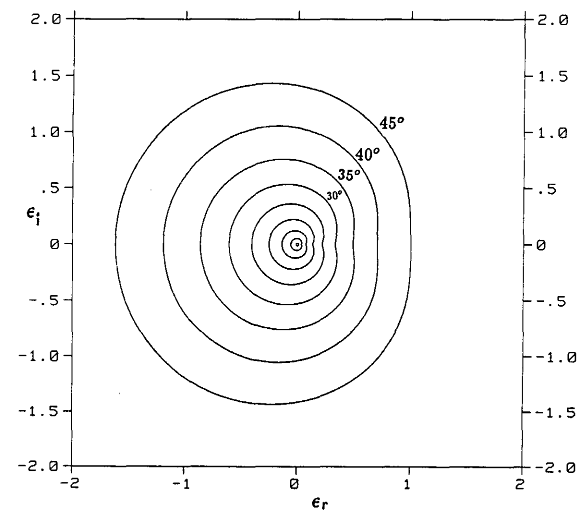

Fig. 1. Contours of constant pseudo-Brewster angle ϕ_{pB} in the complex ϵ plane for angles ϕ_{pB} from 5° to 45° in 5° steps. Each contour is symmetrical with respect to the real axis.

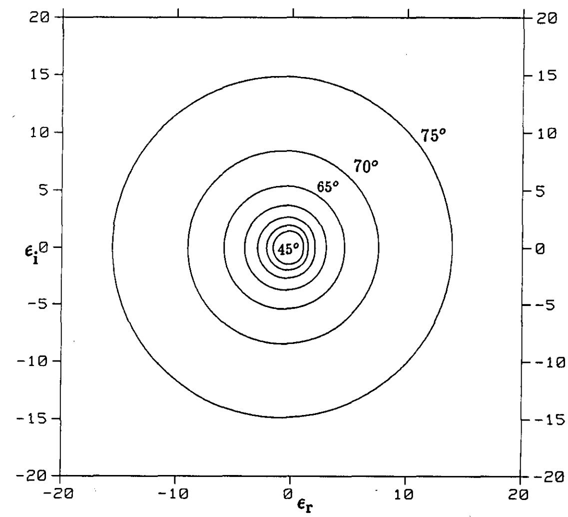

Fig. 2. Continuation of Fig. 1 for angles ϕ_{pB} from 45° to 75° in steps of 5°.

II. Constant Pseudo-Brewster Angle Contours in the Complex ϵ Plane

The equation of the constant pseudo-Brewster angle contour (CPBAC) in the complex ϵ plane takes its simplest form in polar coordinates. For this purpose, we write

$$\epsilon = |\epsilon| \exp(j\theta), \tag{7}$$

where $|\epsilon|$ and θ are the absolute value and argument (or angle) of complex ϵ, respectively. If $\epsilon_r = |\epsilon| \cos\theta$ is substituted into Eq. (5), the result can be reduced to a cubic equation in $|\epsilon|$ of the standard form,

$$|\epsilon|^3 + p|\epsilon| + q = 0, \tag{8}$$

where

$$p = \frac{-u^2(3 - 2u)}{(1 - u)^2}, \tag{9}$$

$$q = q' \cos\theta, \tag{10}$$

$$q' = \frac{2u^3}{(1 - u)^2}, \tag{11}$$

where u is given by Eq. (6). The nature of the roots of cubic Eq. (8) is determined by the discriminant[7]

$$D = (p/3)^3 + (q/2)^2. \tag{12}$$

We have verified that

$$D < 0 \tag{13}$$

for all possible values of $u (0 < u < 1)$ and $\theta (0 \leq \theta \leq \pi)$, but the proof is omitted for brevity. Consequently, Eq. (8) always has three real roots of which only one is positive, hence acceptable. This root is given by[7]

$$|\epsilon| = l \cos(\zeta/3), \tag{14}$$

where

$$l = 2(-p/3)^{1/2}, \tag{15}$$

$$\zeta = \arccos\left[\frac{(-q/2)}{(|p|^3/27)^{1/2}}\right]. \tag{16}$$

From the definitions of p,q [Eqs. (9)–(11)], and u [Eq. (6)], l and ζ can be written explicitly as

$$l = 2 \tan^2\phi_{pB}(1 - \tfrac{2}{3} \sin^2\phi_{pB})^{1/2}, \tag{17}$$

$$\zeta = \arccos[-\cos\theta \cos^2\phi_{pB}(1 - \tfrac{2}{3} \sin^2\phi_{pB})^{-3/2}]. \tag{18}$$

Equation (14), which to our knowledge is new, specifies the CPBAC in polar coordinates in the complex ϵ plane. For a given ϕ_{pB}, $|\epsilon|$ varies with θ as a cosine function of amplitude, l, which is determined by ϕ_{pB} only [Eq. (17)], and argument $\zeta/3$, which is a somewhat complicated function of θ [Eq. (18)].

Equations (14), (17), and (18) permit the direct calculation of the Cartesian coordinates

$$(\epsilon_r,\epsilon_i) = (|\epsilon| \cos\theta, |\epsilon| \sin\theta) \tag{19}$$

of any number of points on the CPBAC for any given ϕ_{pB} (e.g., 181 points are obtained by scanning θ in 1° steps over the range $0 \leq \theta \leq 180°$). This can be repeated for any number of specified angles ϕ_{pB} making possible the accurate plotting of any desired family of CPBACs.

Figure 1 shows a family of CPBACs for ϕ_{pB} from 5° to 45° in steps of 5°. To reveal the nature of these contours, we have allowed θ to scan the range $0° \leq \theta < 360°$, even though complex ϵ is restricted only to the half-plane above (or below[8]) the real axis, the real axis included. It is apparent that a CPBAC for $\phi_{pB} \leq 45°$ has a cardioid shape and departs considerably from a circle centered on the origin. Therefore, the circle approximation[9] is far from satisfactory in this range of ϕ_{pB}.

Figure 2 is a continuation of Fig. 1 in which the CPBACs are plotted for ϕ_{pB} from 45° to 75° in steps of 5°. For $\phi_{pB} > 75°$, the CPBACs become nearly circles centered on the origin, hence are not plotted.

III. Characteristics of the CPBACs

According to Eq. (14), l, which is given by Eq. (17), defines an upper bound on $|\epsilon|$ for a specified or measured ϕ_{pB}. The points of intersection A, B, and C of the CPBAC with the positive real axis ($\theta = 0°$), the imaginary axis ($\theta = 90°$), and the negative real axis ($\theta = 180°$) are also special features that characterize a given contour. The associated values of ϵ are

$$\epsilon_A = \tan^2\phi_{pB}, \tag{20}$$

$$\epsilon_B = j\frac{\sqrt{3}}{2}l, \tag{21}$$

$$\epsilon_C = -\tfrac{1}{2}[\epsilon_A + \sqrt{3}(l^2 - \epsilon^2_A)^{1/2}]. \tag{22}$$

Figure 3 shows a CPBAC in the upper half of the complex ϵ plane, with the points A, B, and C marked. As θ increases from 0° to 180°, the contour is traced in the direction of the arrow from A to B to C, and the associated minimum reflectance $|r_p|_{\min}$ at ϕ_{pB} (which angle is fixed) increases monotonically from 0 (at A) to 1 (at C). [It is obvious that Eq. (20) is the Brewster law: in the limiting case of $\theta = 0°$ (ϵ real), ϕ_{pB} becomes the exact Brewster angle.]

The deviation of a given contour from a circle (or semicircle) centered on the origin is measured by the ratios

$$\eta_1 = |\epsilon_B|/|\epsilon_A| = (3 - 2\sin^2\phi_{pB})^{1/2}, \tag{23}$$

$$\eta_2 = |\epsilon_C|/|\epsilon_A| = \tfrac{1}{2}[1 + (9 - 8\sin^2\phi_{pB})^{1/2}]. \tag{24}$$

A specified or measured ϕ_{pB} places $|\epsilon|$ in the interval $\tan^2\phi_{pB} = |\epsilon_A| \le |\epsilon| \le \eta_2|\epsilon_A|$ but leaves θ unrestricted. The CPBAC deviates most from a (semi)circle as $\phi_{pB} \to 0$; in that limit η_1 and η_2 reach their maximum possible values of $\sqrt{3}$ and 2, respectively. On the other hand, when $\phi_{pB} \to 90°$, η_1 and $\eta_2 \to 1$ and the CPBAC approaches a semicircle.

Even for an angle as high as 75°, the CPBAC is perceptibly different from a centered circle (see Fig. 2). (At $\phi_{pB} = 75°$, $\eta_1 = 1.065$ and $\eta_2 = 1.120$.) Therefore, one should not invoke the circle approximation[9] of the CPBAC except near grazing incidence. (At $\phi = 80°$, $\eta_1 = 1.030$, $\eta_2 = 1.057$; the deviation of the CPBAC from a centered circle is ~5%.)

An interesting question is the following. What is the largest value of ϕ_{pB} for which the CPBAC lies entirely within the unit circle of the complex ϵ plane? Put differently, what is the upper limit on ϕ_{pB} below which the optical constants ϵ_r and ϵ_i are always fractional? The answer is obtained by setting

$$\epsilon_C = -1. \tag{25}$$

Substitution of Eq. (25) into Eq. (22) and solving the resulting equation for ϕ_{pB} give the interesting result:

$$\tan^4\phi_{pB} = \tfrac{1}{3}, \tag{26}$$

hence

$$\phi_{pB} = 37.23°. \tag{27}$$

A measured pseudo-Brewster angle of <37.23° directly indicates that both ϵ_r and ϵ_i are fractional. At this special angle, $\phi_{pB} = 37.23°$, $l = 1.004$, i.e., the amplitude of the cosine function of Eq. (14) happens to be nearly unity.

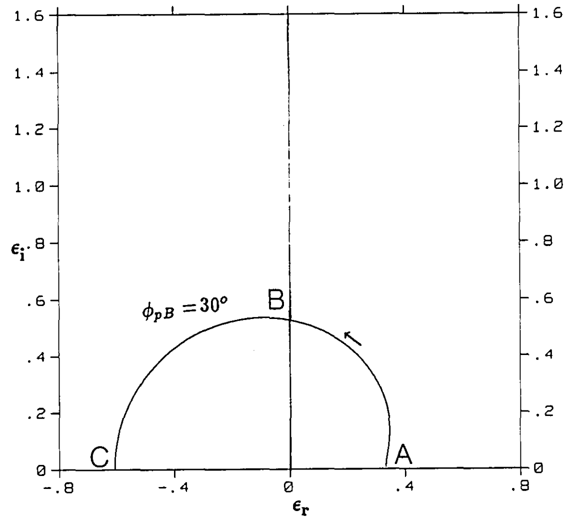

Fig. 3. An iso-ϕ_{pB} contour in the upper half of the complex ϵ plane. A, B, and C are the points of intersection of the contour with the positive real axis, imaginary axis, and negative real axis, respectively. The arrow indicates the direction in which the minimum reflectance (at ϕ_{pB}) increases monotonically from 0 at A to 1 at C.

Another special angle is $\phi_{pB} = 45°$. The polar equation of the associated CPBAC is given for reference:

$$|\epsilon| = (\tfrac{8}{3})^{1/2}\cos\left\{\frac{1}{3}\cos^{-1}\left[-\left(\frac{27}{32}\right)^{1/2}\cos\theta\right]\right\}. \tag{28}$$

A measured $\phi_{pB} > 45°$ guarantees that $|\epsilon| > 1$. In the intermediate interval, $37.23° < \phi < 45°$, the optical constants may or may not be fractional.

For completeness, we conclude this section by giving the explicit Cartesian equation of the CPBAC, which can be derived by algebraic manipulation of Eq. (5). The result is

$$\epsilon_i = [a + (a^2 - b\epsilon_r)^{1/2} - \epsilon_r^2]^{1/2}, \tag{29}$$

where

$$a = u^2(3 - 2u)/(1 - u)^2, \tag{30}$$

$$b = 2u^3/(1 - u)^2. \tag{31}$$

[Note that $a = -p/2$ and $b = q'$, where p and q' are given by Eqs. (9) and (11).] Equation (29) allows the determination of the maximum possible value of ϵ_i that is consistent with a specified or measured ϕ_{pB} (or u). This maximum is located by the condition that

$$\partial\epsilon_i/\partial\epsilon_r|_{u=\text{const}} = 0. \tag{32}$$

Squaring both sides of Eq. (29), taking the derivative with respect to ϵ_r, and setting the result equal to 0 give

$$16b\epsilon_r^3 - 16a^2\epsilon_r^2 + b^2 = 0. \tag{33}$$

Cubic Eq. (33) can be solved explicitly for ϵ_r and the result substituted into Eq. (29) to yield $\epsilon_{i\max}$. The remaining details of this exercise are left to the interested reader.

IV. Determination of the Optical Constants of an Absorbing Medium from the Normal Incidence Reflectance and the Pseudo-Brewster Angle: Graphic Method

Humphreys-Owen[2] and others[5,10,11] surveyed several methods for the determination of optical constants n and k [real and imaginary parts of the complex refractive index N, Eq. (4)] of an absorbing medium from two measured reflection parameters without ellipsometric analysis. Darcie and Whalen[6] (D&W) added a new method which is based on measurement of the normal incidence intensity (power) reflectance R_o and the pseudo-Brewster angle ϕ_{pB} of minimum parallel reflectance. They presented a nomogram of contours of constant n and contours of constant k in the $R_o\phi_{pB}$ plane and a numerical method with which n and k may be determined once R_o and ϕ_{pB} are specified.

We have reexamined the D&W method in the light of our analysis of the nature of the CPBACs. An alternative nomogram is suggested that consists of the iso-R_o contours and the iso-ϕ_{pB} contours in the (complex) nk plane. In Sec. V, we also give an analytical solution that provides a direct answer for (n,k) given a set of measurements (R_o,ϕ_{pB}), without recourse to numerical iteration.

The normal incidence, complex amplitude reflection coefficient is obtained by setting $\phi = 0$ in Eq. (1):

$$r_o = \frac{\epsilon^{1/2} - 1}{\epsilon^{1/2} + 1}, \tag{34}$$

The associated power reflectance is

$$R_o = r_o r_o^*. \tag{35}$$

If we write $\epsilon^{1/2} = N = n + jk$, Eqs. (34) and (35) give the well-known result[5]

$$R_o = \frac{(n-1)^2 + k^2}{(n+1)^2 + k^2}. \tag{36}$$

Equation (36) can be rearranged to read

$$\left(n - \frac{1}{F}\right)^2 + k^2 = G^2, \tag{37}$$

where

$$F = \frac{1 - R_o}{1 + R_o}, \tag{38}$$

$$G = \frac{2R_o^{1/2}}{1 - R_o}. \tag{39}$$

Equation (37) indicates that the iso-R_o contour is a (semi)circle in the nk plane with center on the n axis at $(1/F,0)$ and radius G.

The CPBACs in the nk plane are also analytically determinable from

$$(n,k) = \left(|\epsilon|^{1/2} \cos\frac{\theta}{2}, |\epsilon|^{1/2} \sin\frac{\theta}{2}\right), \tag{40}$$

where $|\epsilon|$ is related to θ at a given ϕ_{pB} by Eq. (14) [and Eqs. (17) and (18)].

Figure 4 shows a family of iso-R_o contours (circle arcs) and iso-ϕ_{pB} contours (CPBACs) in the nk plane.

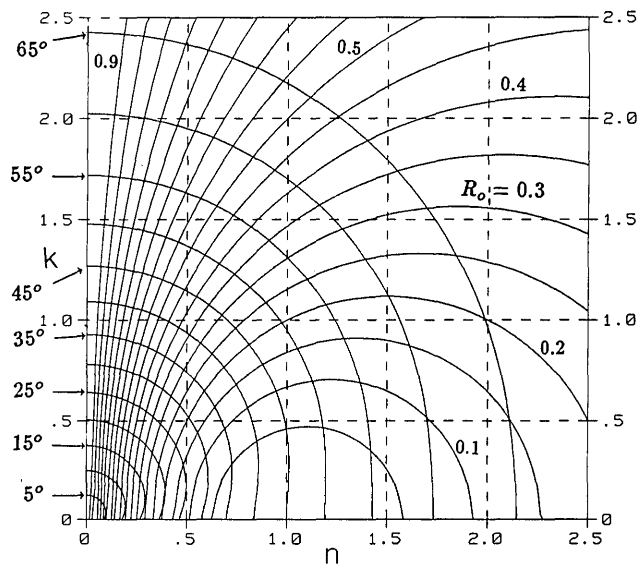

Fig. 4. Families of iso-R_o and iso-ϕ_{pB} contours in the nk plane. R_o is the normal incidence reflectance and assumes values from 0.05 to 0.90 in steps of 0.05. ϕ_{pB} is the pseudo-Brewster angle and takes values from 5° to 65° in steps of 5°. This nomogram can be used to find an approximate solution for the optical constants (n,k) given a measured set (R_o,ϕ_{pB}).

The nomogram is limited to the square $0 \le n,k \le 2.5$ and covers the range of ϕ_{pB} from 5 to 65° in steps of 5° and of R_o from 0.05 to 0.90 in steps of 0.05. The major advantage of this type of nomogram is that both families of iso-R_o and iso-ϕ_{pB} contours are governed by explicit equations (with the iso-R_o contours being circles). Thus we have provided the reader with the analytical tools with which he or she can generate an accurate version of the nomogram with a computer and a plotter. The values and ranges of R_o and ϕ_{pB} are selected at will.

Figure 5 is another nomogram of iso-R_o, iso-ϕ_{pB} contours plotted over a large range of n,k, a square of side 20. The constant values of R_o are the same as before (0.05–0.90 in steps of 0.05) and the constant values of ϕ_{pB} are 65°, 70°, 73°, 77°, 79°, and 80–87° in steps of 1°.

In general, an iso-R_o contour intersects an iso-ϕ_{pB} contour at one and only one point, so that a unique solution (n,k) is found for a given pair (R_o,ϕ_{pB}) as shown in Fig. 6. An important exception occurs when n and k become fractional, as in Fig. 4. Here an iso-R_o contour may intersect an iso-ϕ_{pB} contour at two points leading to two solution pairs (n,k) that are consistent with one and the same measured set (R_o,ϕ_{pB}). This is the case, for example, when $R_o = 0.20$ and $\phi_{pB} = 20°$. For clarity, the intersection of the $R_o = 0.20$ and $\phi_{pB} = 20°$ contours in the nk plane (at the two points P_1 and P_2) is illustrated in Fig. 7 on an expanded scale. The possibility of multiple solutions was not discussed in Ref. 6, because the domain of fractional optical constants was not covered.

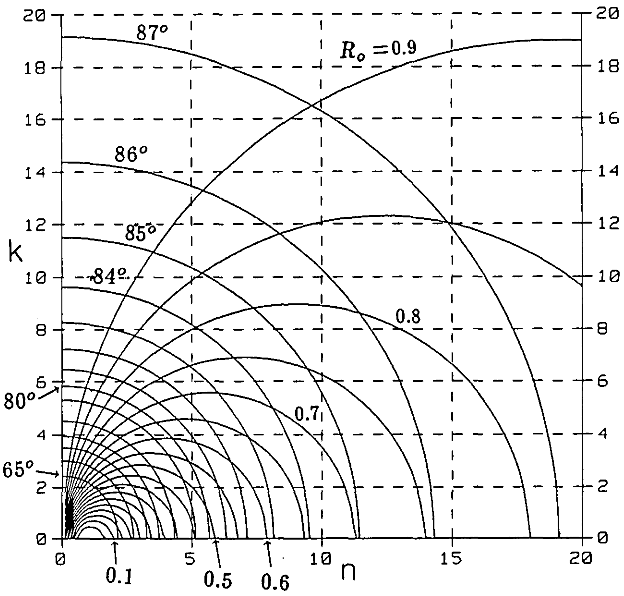

Fig. 5. Similar to Fig. 4 except that the constant values of ϕ_{pB} are 65°, 70°, 73°, 75°, 77°, 79°, and 80–87° in steps of 1°. (R_o is in the range from 0.05 to 0.90 in steps of 0.05, as in Fig. 4). Again this nomogram serves as an aid in solving the $(R_o,\phi_{pB}) \rightarrow (n,k)$ inversion problem.

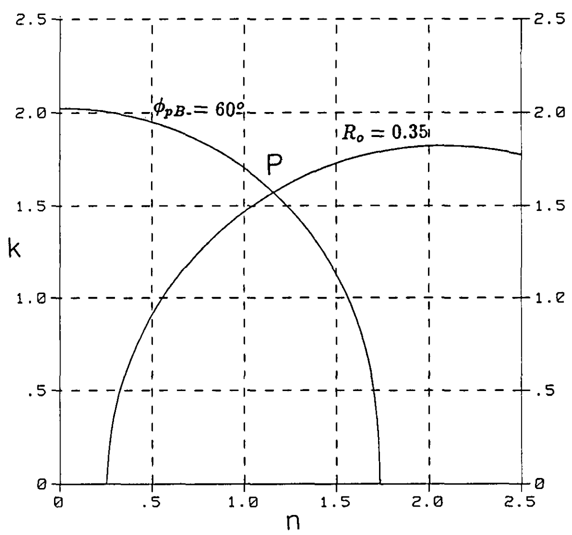

Fig. 6. An iso-R_o contour (R_o = 0.35) generally intersects an iso-ϕ_{pB} contour (ϕ_{pB} = 60°) at one point P that specifies a unique solution pair (n,k) at P.

V. Determination of the Optical Constants of an Absorbing Medium from the Normal-Incidence Reflectance and the Pseudo-Brewster Angle: Analytical Solution

If Eq. (34) is substituted into Eq. (35) and F of Eq. (35) is evaluated, one gets

$$F = \frac{2\,\mathrm{Re}\,\epsilon^{1/2}}{|\epsilon| + 1} = \frac{2|\epsilon|^{1/2}\cos\frac{\theta}{2}}{|\epsilon| + 1}, \qquad (41)$$

where $\epsilon = |\epsilon|\exp(j\theta)$, as before. Equation (41) can be solved for $\cos(\theta/2)$:

$$\cos(\theta/2) = \tfrac{1}{2}(|\epsilon|^{1/2} + |\epsilon|^{-1/2})F. \qquad (42)$$

Equation (42) is one form of the constraint on $|\epsilon|$ and θ for a given F (or R_o).[12] Squaring both sides of Eq. (42) and using the trigonometric identity $\cos\theta = 2\cos^2(\theta/2) - 1$, we obtain

$$2\cos\theta = (|\epsilon| + |\epsilon|^{-1} + 2)F^2 - 2. \qquad (43)$$

The condition of minimum parallel reflectance (at ϕ_{pB}) establishes another relationship (or constraint) between $|\epsilon|$ and $\cos\theta$. This appears in Eq. (8), where p and q are given by Eqs. (9)–(11). Solving Eq. (8) for $\cos\theta$, we find that

$$2\cos\theta = u^{-1}(3 - 2u)|\epsilon| - u^{-3}(1 - u)^2|\epsilon|^3. \qquad (44)$$

By equating the right-hand sides of Eqs. (43) and (44), $\cos\theta$ is eliminated and a quartic equation in $|\epsilon|$ only is obtained:

$$\sum_{i=0}^{4} \beta_i|\epsilon|^i = 0, \qquad (45)$$

where

$$\begin{aligned} \beta_0 &= u^3F^2, \\ \beta_1 &= 2u^3(F^2 - 1), \\ \beta_2 &= u^2(uF^2 + 2u - 3), \\ \beta_3 &= 0, \\ \beta_4 &= (1 - u)^2. \end{aligned} \qquad (46)$$

For given R_o and ϕ_{pB}, the coefficients β_i of Eqs. (46) are determined. [Recall that $u = \sin^2\phi_{pB}$ and $F = (1 - R_o)/(1 + R_o)$.] Quartic Eq. (45) has a direct (closed-form) solution.[13] Only those roots that are real and positive are acceptable. Once $|\epsilon|$ is found, $\cos\theta$ can be calculated from Eq. (43) and the real and imaginary parts of complex ϵ are subsequently obtained:

$$\epsilon_r = |\epsilon|\cos\theta = \tfrac{1}{2}(|\epsilon| + 1)^2F^2 - |\epsilon|, \qquad (47)$$

$$\epsilon_i = |\epsilon|\sin\theta = (|\epsilon|^2 - \epsilon_r^2)^{1/2}; \qquad (48)$$

n and k follow from Eq. (40) or by taking the complex square root. This concludes the development of the analytical method of determining the optical constants n,k from the measurements of R_o,ϕ_{pB}.

Our analytical method has been tested using simulated data[14] and the data given by D&W, and has been found to yield the correct results. To quote one specific numerical example, we take an InSb semiconductor substrate. At wavelength λ = 517 nm, D&W give R_o = 0.46 and ϕ_{pB} = 77.13°. For this (R_o,ϕ_{pB}) pair, Eq. (45) [with the coefficients calculated from Eqs. (46)] yields the following four real roots: 19.6512, 0.0759, −1.7840, and −17.9431. Of these four roots, the last two are negative and are rejected because $|\epsilon| > 0$. The second is also rejected because it is inconsistent with (the large) ϕ_{pB}; only the first root $|\epsilon|$ = 19.6512 is acceptable. Continuing with the analytical solution, we get $\cos\theta$ = 0.4844 (hence θ = 61.026°), ϵ_r = 9.5192, ϵ_i = 17.1917, and n = 3.8191 and k = 2.2508. The latter n and k agree with the values of D&W.

As another use of our analytical method, we determine the exact points of intersections P_1 and P_2 of the $R_o = 0.20$ and $\phi_{pB} = 20°$ contours in the nk plane (Fig. 7). Quartic Eq. (45) gives the following four roots: $|\epsilon| = 0.1776, 0.1517, -0.1646$, and -0.1646. Both positive roots are acceptable in this case and the analytical solution fixes the exact coordinates (n,k) of points P_1 (0.3925,0.1534) and P_2 (0.3839,0.0657). A significant advantage of the $(R_o,\phi_{pB}) \rightarrow (n,k)$ analytical inversion method presented here is that it facilitates the study of the propagation of experimental errors $(\delta R_o,\delta\phi_{pB})$ into corresponding errors $(\delta n,\delta k)$ in the determined optical constants. For example, using our approach, we have verified directly the uncertainties $\delta n,\delta k$ caused by $\delta R_o = \pm 0.001$ and $\delta\phi_{pB} = \pm 0.05°$ for the cases studied by D&W.

VI. Determination of the Optical Constants of an Absorbing Medium from the Measurement of Two Pseudo-Brewster Angles

Elsewhere Azzam[15] has described a novel analytical method for the determination of ϵ_r and ϵ_i (hence n and k) of an absorbing medium from the pseudo-Brewster angles ϕ_{pB1} and ϕ_{pB2} measured in two different transparent media of incidence of dielectric constants ϵ_{o1} and ϵ_{o2}. Here we provide further (graphic) insight into this two-angle method (TAM) by making use of the results of Sec. II which resolved the nature of the iso-ϕ_{pB} contours in the complex ϵ plane. We do this by way of the specific example given in Ref. 15, namely, that of an opaque TiN film deposited on a Cleartran (ZnS) substrate. The two pseudo-Brewster angles ϕ_{pB1} and ϕ_{pB2} are measured from the air side ($\epsilon_{o1} = 1$) and the substrate side ($\epsilon_{o2} = n^2_{ZnS}$) of the TiN film. The (simulated) measurements (using published values of the optical constants of TiN and ZnS) yield $\phi_{pB1} = 66.4323°$ and $\phi_{pB2} = 40.1148°$ at wavelength $\lambda = 600$ nm.

Figure 8 shows the two CPBACs in the complex ϵ plane at these two angles as determined by Eq. (14). The task of determining complex ϵ from ϕ_{pB1} and ϕ_{pB2} amounts to finding the radial line through the origin ($\arg\epsilon = \theta =$ constant) at which

$$|\epsilon_1|/|\epsilon_2| = \epsilon_{o2}/\epsilon_{o1}, \tag{49}$$

where, for the present example,

$$\epsilon_{o2}/\epsilon_{o1} = n^2_{ZnS} = 2.363^2 = 5.583769. \tag{50}$$

The left-hand size of Eq. (49) is a function of θ only given by

$$|\epsilon_1|/|\epsilon_2| = f_{12}(\theta) = \frac{l_1 \cos(\zeta_1/3)}{l_2 \cos(\zeta_2/3)}, \tag{51}$$

where l_i and ζ_i ($i = 1,2$) are the values of l and ζ evaluated from Eqs. (17) and (18), respectively, at ϕ_{pB1} and ϕ_{pB2}. Subscript 12 of $f_{12}(\theta)$ is used to emphasize the dependence of this function of θ on the two angles. Combining Eqs. (49)–(51) gives

$$f_{12}(\theta) = \epsilon_{o2}/\epsilon_{o1}, \tag{52}$$

or

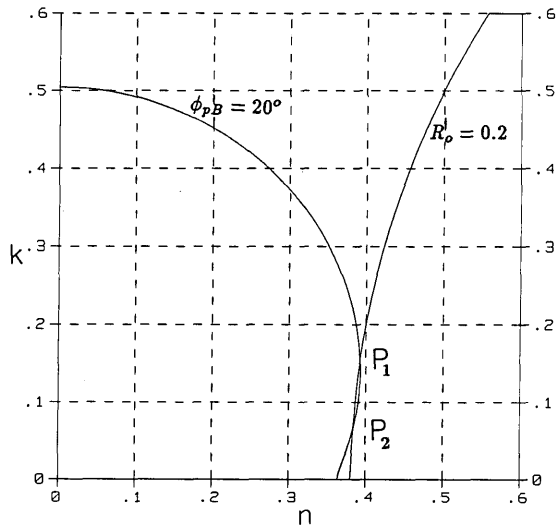

Fig. 7. In the domain of fractional optical constants, an iso-R_o contour ($R_o = 0.20$) may intersect an iso-ϕ_{pB} contour ($\phi_{pB} = 20°$) at two points P_1 and P_2 that specify two valid solution pairs (n,k) at P_1 and P_2.

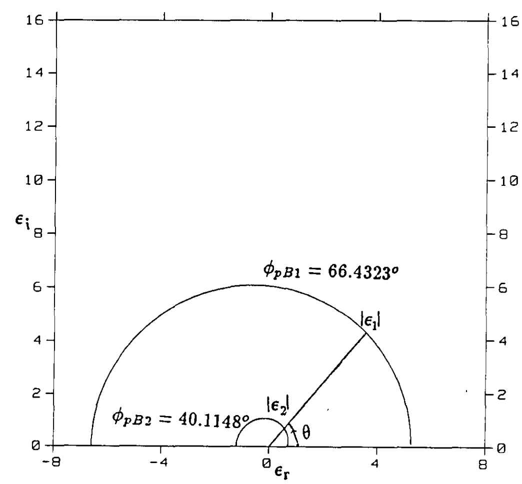

Fig. 8. Two iso-ϕ_{pB} contours at $\phi_{pB} = 66.4323°$ and $\phi_{pB} = 40.1148°$ in the complex ϵ plane. These two angles are the pseudo-Brewster angles measured in external (in air) and internal reflection, respectively, on an opaque TiN film covering a ZnS substrate at $\lambda = 600$ nm. Finding complex ϵ of the TiN film amounts to locating a radial straight line through the origin (shown dashed) such that $|\epsilon_1|/|\epsilon_2| = 2.363^2$ where $n = 2.363$ is the refractive index of the ZnS substrate at 600 nm.

$$f_{12}(\theta) = 5.583769. \tag{53}$$

Figure 9 shows a graph of $f_{12}(\theta)$ vs θ for $\phi_{pB1} = 66.4323°$ and $\phi_{pB2} = 40.1148°$, which is the example at hand. The solution of Eq. (53) for θ is represented by the intersection of the curve of $f_{12}(\theta)$ with a horizontal straight line at an ordinate equal to 5.583769. This fixes θ (= 125.856° by numerical iteration) and determines the correct value of complex $\epsilon_1 = \epsilon_{TiN} = (-3.740,5.175)$ at $\lambda = 600$ nm by Eq. (14).

The method presented in this section is not meant to substitute for the direct and explicit analytical method of Ref. 15.

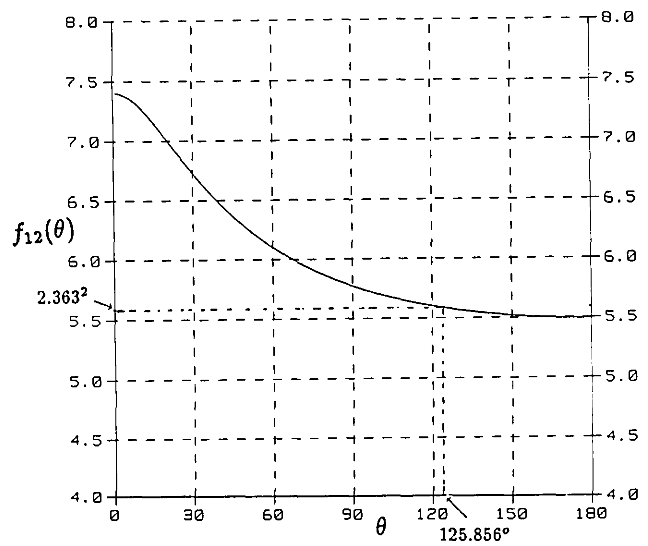

Fig. 9. Function $f_{12}(\theta)$ of Eq. (51) plotted vs θ for the pseudo-Brewster angles of external and internal reflection, $\phi_{pB1} = 66.4323°$ and $\phi_{pB2} = 40.1148°$, of a TiN film on a ZnS substrate. The point of intersection of the curve with a horizontal line drawn at an ordinate $= 2.363^2$ gives the argument $\theta(= 125.856°)$ of complex ϵ of the TiN film.

VII. Summary

The following is a brief summary of what is accomplished in this paper:

(1) A polar equation $|\epsilon|\ l \cos(\zeta/3)$ has been derived to represent the locus of all points in the complex ϵ plane that share the same pseudo-Brewster angle ϕ_{pB} of minimum parallel reflectance. In this equation, l is a function of ϕ_{pB} and ζ is a function of ϕ_{pB} and θ, where θ is the (polar) angle of $\epsilon(\theta = \arg\epsilon)$. Families of iso-$\phi_{pB}$ contours are presented. It is noted that these contours deviate significantly from circles centered at the origin, except near grazing incidence. $\phi_{pB} < 37.23°$ indicates fractional optical constants (i.e., $|\epsilon| < 1$), whereas $\phi_{pB} > 45°$ guarantees that $|\epsilon| > 1$. Exact limits have been set on $|\epsilon|$ for a given value of ϕ_{pB}.

(2) A method for the determination of the optical constants n,k from measurements of the normal incidence reflectance R_o and the pseudo-Brewster angle ϕ_{pB} has been examined in detail. Nomograms that consist of families of iso-R_o and iso-ϕ_{pB} contours in the complex nk plane are presented. The reader is given the mathematical equations with which to produce his or her own version of the nomogram, e.g., to facilitate the application of the $R_o - \phi_{pB}$ method to a certain class of materials such as semiconductors. We have noted that two solution sets of (n,k) can correspond to the same measurement set (R_o,ϕ_{pB}) in the domain of fractional optical constants.

(3) An analytical solution for the $(R_o,\phi_{pB}) \rightarrow (n,k)$ inversion problem has been discovered. It involves solving a quartic equation in $|\epsilon|$ whose coefficients are determined by R_o and ϕ_{pB}. This analytical solution facilitates error analysis and makes the $R_o - \phi_{pB}$ method more attractive to use.

(4) A new method for measuring optical constants that uses two pseudo-Brewster angles measured in two different media of incidence[15] is further discussed based on our understanding of the nature of the iso-ϕ_{pB} contours. The associated inverse problem is reformulated with the help of a graphic construction.

This work was supported in part by the National Science Foundation.

References

1. See, for example, R. M. A. Azzam and N. M. Bashara, *Ellipsometry and Polarized Light* (North-Holland, Amsterdam, 1987).
2. S. P. F. Humphreys-Owen, "Comparison of Reflection Methods for Measuring Optical Constants without Polarimetric Analysis, and Proposal for New Methods Based on the Brewster Angle," Proc. Phys. Soc. London **77**, 949–957 (1961).
3. R. M. A. Azzam, "Maximum Minimum Reflectance of Parallel-Polarized Light at Interfaces between Transparent and Absorbing Media," J. Opt. Soc. Am. **73**, 959–962 (1983).
4. S. Y. Kim and K. Vedam, "Analytic Solution of the Pseudo-Brewster Angle," J. Opt. Soc. Am. A **3**, 1772–1773 (1986).
5. H. B. Holl, "Specular Reflection and Characteristics of Reflected Light," J. Opt. Soc. Am. **57**, 683–690 (1967).
6. T. E. Darcie and M. S. Whalen, "Determination of Optical Constants using Pseudo-Brewster Angle and Normal-Incidence Reflectance Measurements," Appl. Opt. **23**, 1130–1131 (1984).
7. See, for example, S. M. Selby, Ed., *Standard Mathematical Tables* (Chemical Rubber Co., Cleveland, OH, 1972), pp. 103–105.
8. This depends on whether the $\exp(j\omega t)$ or $\exp(-j\omega t)$ time dependence of a time-harmonic wave field is assumed. See R. H. Muller, "Definitions and Conventions in Ellipsometry," Surf. Sci. **16**, 14–33 (1969).
9. J. M. Bennett and H. E. Bennett, "Polarization," in *Handbook of Optics*, W. G. Driscoll and W. Vaughan, Eds. (McGraw-Hill, New York, 1978).
10. W. R. Hunter, "Measurement of Optical Properties of Materials in the Vacuum Ultraviolet Spectral Region," Appl. Opt. **21**, 2103–2114 (1982).
11. R. M. A. Azzam, "Explicit Determination of the Complex Refractive Index of an Absorbing Medium from Reflectance Measurements at and Near Normal Incidence," J. Opt. Soc. Am. **72**, 1439–1440 (1982), and references cited therein.
12. A symmetrical and more interesting form of this constraint is obtained by defining the parameter $\alpha = \ln|\epsilon|$; so that $|\epsilon| = \exp(\alpha)$. This transforms Eq. (42) to $\cosh(\alpha/2) = (1/F)\cos(\theta/2)$. This is perhaps the simplest and most elegant form of the polar equation of the iso-R_o contour in the complex ϵ plane.
13. See, e.g., S. M. Selby, Ed., *Standard Mathematical Tables* (Chemical Rubber Co., Cleveland, OH, 1972), p. 106.
14. We start with a given pair of optical constants (n,k) [or (ϵ_r,ϵ_i)] and solve Eq. (5) for ϕ_{pB} and use Eq. (36) to calculate R_o. With our analytical inversion procedure, we work backward to determine (n,k) from the (R_o,ϕ_{pB}) set. The same (n,k) pair that we started with is obtained in a self-consistent manner.
15. R. M. A. Azzam, "Analytical Determination of the Complex Dielectric Function of an Absorbing Medium from Two Angles of Incidence of Minimum Parallel Reflectance," J. Opt. Soc. Am. A **6**, 1213–1216 (1989).