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Ellipsometric function of a film-substrate system: Applications to the design of reflection-type optical devices and to ellipsometry*

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The ratio $\rho = R_p/R_s$ of the complex amplitude-reflection coefficients R_p and R_s for light polarized parallel (p) and perpendicular (s) to the plane of incidence, reflected from an optically isotropic film-substrate system, is investigated as a function of the angle of incidence ϕ and the film thickness d . Both constant-angle-of-incidence contours (CAIC) and constant-thickness contours (CTC) of the ellipsometric function $\rho(\phi, d)$ in the complex ρ plane are examined. For transparent films, $\rho(\phi, d)$ is a periodic function of d with period D_ϕ that is a function of ϕ . For a given angle of incidence ϕ and film thickness d ($0 \leq \phi \leq 90, 0 \leq d < D_\phi$), the equispaced linear array of points $(\phi, d + m D_\phi)$ ($m = 0, 1, 2, \dots$) in the real (ϕ, d) plane is mapped by the periodic function $\rho(\phi, d)$ into one distinct point in the complex ρ plane. Conversely, for a given film-substrate system, any value of the ellipsometric function ρ can be realized at one particular angle of incidence ϕ and an associated infinite series of film thicknesses $d, d + D_\phi, d + 2D_\phi, \dots$. This analysis leads to (1) a unified scheme for the design of all reflection-type optical devices, such as polarizers and retarders, (2) a novel null ellipsometer without a compensator, for the measurement of films whose thicknesses are within certain permissible ranges, and (3) an inversion procedure for the nonlinear equations of reflection ellipsometry that separates the determination of the optical constants (refractive indices and extinction coefficients) of the film and substrate from the film thickness. Extension of the work to absorbing films is discussed.

Index Headings: Ellipsometry; Reflection; Polarization; Films.

We consider the case of light reflection by a substrate covered by a single film. As shown in Fig. 1, the film of thickness d has parallel plane boundaries and is sandwiched between semi-infinite ambient and substrate media. The ambient (medium 0), the film (medium 1), and the substrate (medium 2) are all homogeneous and optically isotropic with refractive indices N_0, N_1 , and N_2 , respectively. The complex amplitude-reflection coefficients R_p and R_s for light polarized with its electric vector vibrating parallel (p) and perpendicular (s) to the plane of incidence are given by

$$R_\nu = \frac{r_{01\nu} + r_{12\nu} e^{-j2\beta}}{1 + r_{01\nu} r_{12\nu} e^{-j2\beta}}, \quad \nu = p, s \quad (1)$$

where $r_{01\nu}$ and $r_{12\nu}$ are the ambient-film (0-1) and film-substrate (1-2) interface Fresnel reflection coefficients for the two fundamental polarizations, $\nu = p$ and $\nu = s$. The film phase thickness β is given by

$$\beta = 2\pi(d/\lambda)(N_1^2 - N_0^2 \sin^2 \phi_0)^{1/2}, \quad (2)$$

where λ is the free-space wavelength of light and ϕ_0 is the angle of incidence in medium 0. The ellipsometric function ρ is defined as the ratio^{1,2}

$$\rho = R_p/R_s, \quad (3)$$

of the p and s complex amplitude-reflection coefficients. The ellipsometric function ρ is usually written as

$$\rho = \tan \psi e^{j\Delta}, \quad (4)$$

where $\tan \psi$ is the p -to- s relative amplitude attenuation and Δ is the p -to- s relative phase shift upon reflection. From Eqs. (1) and (3), we obtain

$$\rho = \frac{r_{01p} + r_{12p} e^{-j2\beta}}{1 + r_{01p} r_{12p} e^{-j2\beta}} \times \frac{1 + r_{01s} r_{12s} e^{-j2\beta}}{r_{01s} + r_{12s} e^{-j2\beta}}. \quad (5)$$

The purpose of this paper is to study the behavior of the ellipsometric function ρ for a given ambient-film-

substrate system with known refractive indices N_0, N_1 , and N_2 as a function of its two remaining arguments, the angle of incidence $\phi (= \phi_0)$ and the film thickness d . The formulation provides a unified framework for the design of all reflection-type film-substrate optical devices, such as polarizers and retarders. In addition, the analysis of this paper leads to a novel null ellipsometer without a compensator that is applicable, in general, when the film thickness is of the order of a wavelength or more. It also points the way to an inversion procedure of the nonlinear equations of reflection ellipsometry that promises to be efficient, rapidly convergent, and accurate.

For simplicity, we assume the ambient to be air ($N_0 = 1$), which is usually the case. We initially consider transparent films and later discuss the effect of absorption. Also we take the Si-SiO₂ system, which is technologically important, as an example and assume the light source to be the widely available 6328 Å He-Ne laser. At $\lambda = 6328$ Å, the refractive indices of SiO₂ and Si are 1.46 and 3.85 - $j0.02$, respectively.³

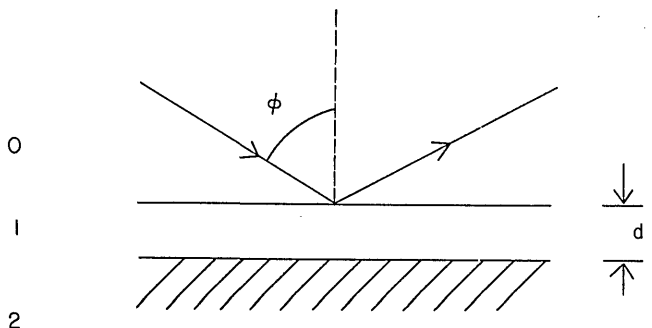


FIG. 1. Film-substrate system. Medium 0 is the ambient, 1 is the film, and 2 is the substrate.

I. CONSTANT-ANGLE-OF-INCIDENCE CONTOURS (CAIC) OF THE ELLIPSOMETRIC FUNCTION $\rho(\phi, d)$

Equations (1) can be cast in the form

$$R_p = \frac{a + bX}{1 + abX}, \quad R_s = \frac{c + dX}{1 + cdX}, \quad (6)$$

and subsequently Eq. (5) becomes

$$\rho = \frac{(a + bX)(1 + cdX)}{(1 + abX)(c + dX)}, \quad (7)$$

or

$$\rho = \frac{A + BX + CX^2}{D + EX + FX^2}. \quad (8)$$

In Eqs. (6)–(8), we have

$$X = e^{-j2\beta}, \quad (9)$$

$$(a, b) = (r_{01p}, r_{12p}), \quad (c, d) = (r_{01s}, r_{12s}), \quad (10)$$

and

$$A = a, \quad B = (b + acd), \quad C = bcd, \quad (11)$$

$$D = c, \quad E = (d + abc), \quad F = abd.$$

Equations (6) show that each of the complex amplitude-reflection coefficients R_p and R_s is related to the complex exponential function of film thickness X , Eq. (9), by a bilinear transformation with coefficients determined by the 0–1 and 1–2 interface Fresnel reflection coefficients,⁴ Eqs. (10). Equation (8) shows that the ratio of the p and s reflection coefficients ρ is a rational function of X in the form of a quadratic divided by another quadratic with coefficients determined by the interface Fresnel reflection coefficients, Eqs. (10) and (11).

If we substitute the film phase thickness β from Eq. (2) into Eq. (9) and set $N_0 = 1$ and $\phi_0 = \phi$, the complex exponential function X becomes

$$X = \exp[-j4\pi(d/\lambda)(N_1^2 - \sin^2\phi)^{1/2}],$$

or

$$X = \exp[-j2\pi(d/D_\phi)], \quad (12)$$

where

$$D_\phi = \frac{\lambda}{2}(N_1^2 - \sin^2\phi)^{-1/2}. \quad (13)$$

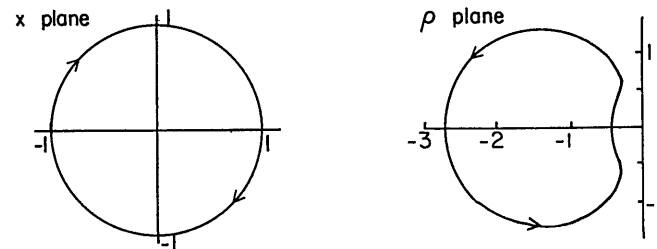


FIG. 2. Left: The unit circle in the complex X plane. Right: Constant-angle-of-incidence contour (CAIC) of the ellipsometric function ρ at an angle of incidence $\phi = 60^\circ$ for Si–SiO₂ system at a wavelength $\lambda = 6328 \text{ \AA}$.

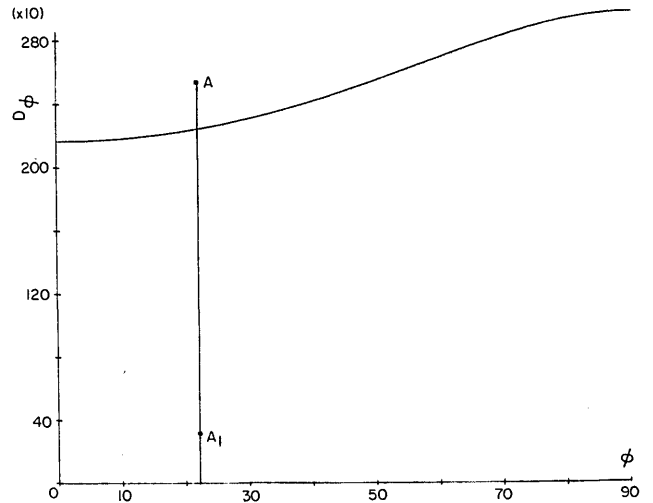


FIG. 3. Thickness period D_ϕ in angstroms for SiO₂ film ($N_1 = 1.46$) at $\lambda = 6328 \text{ \AA}$ as a function of the angle of incidence ϕ , where ϕ is in degrees. Point $A \equiv (\phi, d)$ can be brought down vertically, at the same ϕ , into point $A_1 \equiv (\phi, d - D_\phi)$ that realizes the same ellipsometric function ρ as point A , at a different film thickness $(d - D_\phi)$.

For transparent films, N_1 and D_ϕ are real. In this case, at any angle of incidence ϕ , it can be seen from Eq. (12) that the representative point of the complex exponential function X moves uniformly in a clockwise direction around the unit circle in the complex X plane, as the film thickness d is increased, starting from the point $X = 1$ when $d = 0$, Fig. 2 (left). Note that X is a periodic function of d , so that the unit circle is cyclically traversed. The first full revolution around the unit circle is completed as the film thickness sweeps the interval or period

$$0 \leq d < D_\phi. \quad (14)$$

The thickness period D_ϕ , Eq. (13), is a function of the angle of incidence ϕ that is completely determined by the wavelength λ and the film refractive index N_1 . Figure 3 shows a plot of the thickness period D_ϕ versus the angle of incidence ϕ when $\lambda = 6328 \text{ \AA}$ and $N_1 = 1.46$, which corresponds to the SiO₂ film. The minimum value of D_ϕ occurs at $\phi = 0^\circ$, $D_\phi = 2167.13 \text{ \AA}$, whereas the maximum value occurs at $\phi = 90^\circ$, $D_\phi = 2974.34 \text{ \AA}$.

Because the ellipsometric function ρ is related to the complex exponential X by an analytic rational function of X , Eq. (8), the representative point of ρ must trace a closed contour in the complex ρ plane as X traces the unit circle in the complex X plane (when the film thickness d is increased at a given angle of incidence ϕ).

Figure 2 (right) shows such a constant-angle-of-incidence contour⁵ (CAIC) when $\phi = 60^\circ$ for the Si–SiO₂ system at $\lambda = 6328 \text{ \AA}$. As ϕ scans its entire range

$$0 \leq \phi \leq 90^\circ, \quad (15)$$

the coefficients of the rational function $\rho(X)$, and the period D_ϕ , change so that a whole family of nonintersecting constant- ϕ (variable- d) contours is generated to fill the entire space of the complex ρ plane. Figure 4 shows such a family for the Si–SiO₂ system at $\lambda = 6328 \text{ \AA}$. The

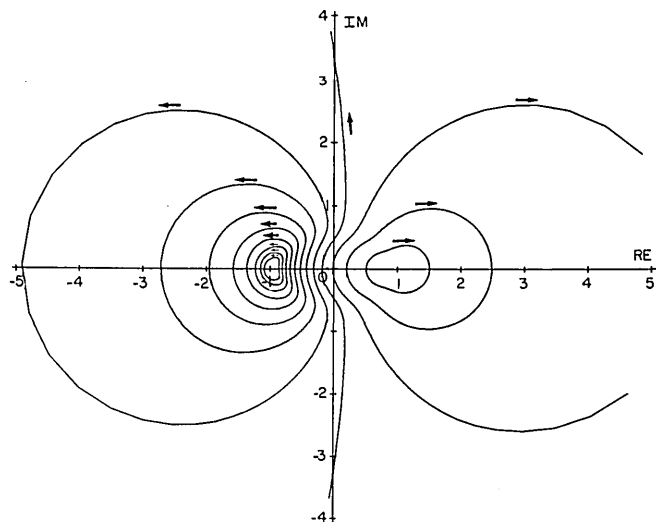


FIG. 4. Constant-angle-of-incidence contours (CAIC's) in the complex ρ plane for Si-SiO₂ system at $\lambda = 6328 \text{ \AA}$ starting near $\rho = -1$ at an angle of incidence $\phi = 30^\circ$ with a step of 5° . On each contour, the arrow indicates the direction in which the film thickness increases.

$\phi = 0^\circ$ (normal incidence) and $\phi = 90^\circ$ (grazing incidence) contours collapse to the null points $\rho = -1$ and $\rho = +1$ on the real axis because, at these angles, $R_p = -R_s$ and $R_p = R_s$, respectively, for any film thickness. All CAIC's that correspond to angles of incidence in a certain range

$$0 < \phi < \phi_s, \tag{16a}$$

enclose the point $\rho = -1$, whereas the remaining contours that correspond to

$$\phi_s < \phi < 90^\circ, \tag{16b}$$

enclose the point $\rho = +1$. The direction in which the thickness increases is indicated by an arrow on each contour. Arrows on all CAIC's enclosing $\rho = -1$ point the same way and opposite to the arrows on all the other contours enclosing $\rho = +1$. The angle of incidence ϕ_s that appears in inequalities (16) leads to a CAIC that passes through the point at infinity. This means that, at this angle, a value (or a set of values equally spaced by the period D_{ϕ_s}) of film thickness can be found such that $\rho = \infty$. Under such conditions, the film-substrate system acts as an *s*-suppressing reflection polarizer. The parameters of such a polarizer will be obtained in Sec. III. The locus of points on the CAIC's where the film thickness is zero, $d = 0$, is the same as the locus of

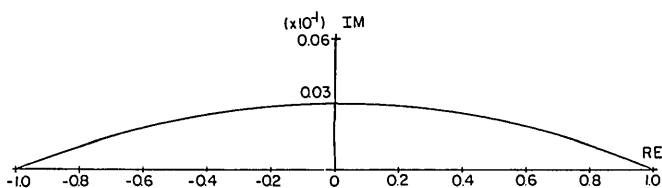


FIG. 5. Zero-thickness contour (ZTC) in the complex ρ plane for Si-SiO₂ system at $\lambda = 6328 \text{ \AA}$.

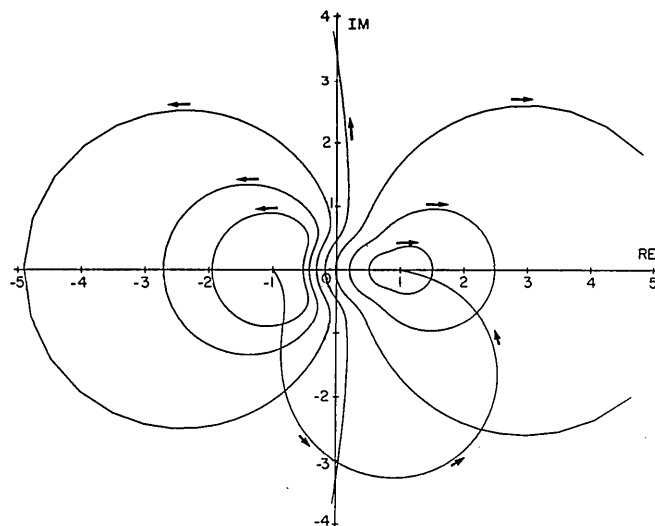


FIG. 6. A constant-thickness contour (CTC) for a film thickness $d = 0.24 \mu\text{m}$ superimposed on the constant-angle-of-incidence contours of $\phi = 55^\circ$ to $\phi = 85^\circ$, with a step of 5° , in the complex ρ plane for Si-SiO₂ system at $\lambda = 6328 \text{ \AA}$.

$$\rho = \rho_{02} = r_{02p} / r_{02s}, \tag{17}$$

which is the ratio of the Fresnel reflection coefficients of the ambient-substrate interface. Because of the low absorption of Si at 6328 \AA , the bare-substrate zero-thickness contour (ZTC) is almost coincident with the straight-line segment from $\rho = -1$ to $\rho = +1$ through the origin. This contour is shown on an expanded scale in Fig. 5.

II. CONSTANT-THICKNESS CONTOURS (CTC) OF THE ELLIPSOMETRIC FUNCTION $\rho(\phi, d)$

The bare-substrate zero-thickness contour, which is shown in Fig. 5, is one member of a complementary family of constant-thickness contours (CTC) that can be drawn in the complex ρ plane. For any given value of film thickness d , the associated CTC can be generated from the zero-thickness contour (ZTC) with the help of

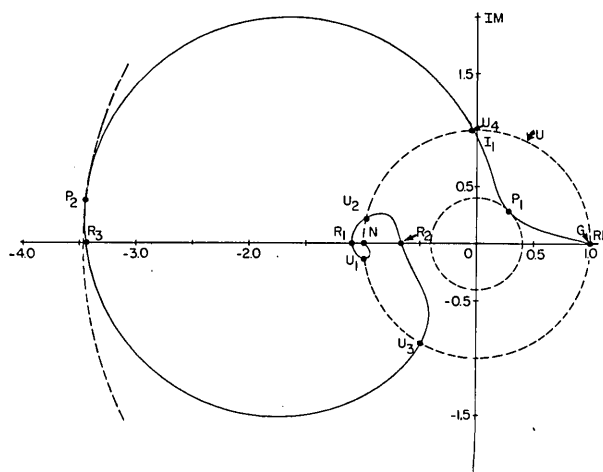


FIG. 7. Constant-thickness contour (CTC) in the complex ρ plane for Si-SiO₂ system at $\lambda = 6328 \text{ \AA}$ and film thickness $d = 1.5 \mu\text{m}$.

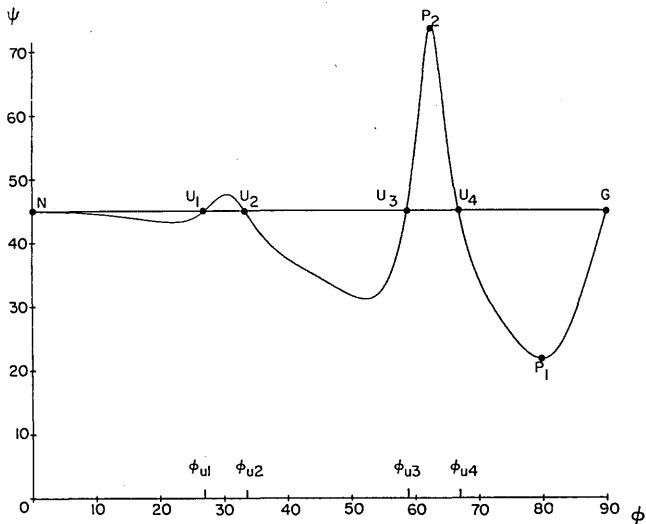


FIG. 8. The angle ψ as a function of the angle of incidence ϕ for Si-SiO₂ system at $\lambda = 6328 \text{ \AA}$ and film thickness $d = 1.5 \mu\text{m}$. Both ψ and ϕ are in degrees.

the constant-angle-of-incidence contours (CAIC) of Fig. 4. Each point on the ZTC corresponds to one angle of incidence ϕ and, as ϕ is increased from $\phi = 0^\circ$ to $\phi = 90^\circ$, we move along the ZTC once from $\rho = -1$ to $\rho = +1$. At a given angle of incidence ϕ , a point on the ZTC can be moved around the constant ϕ contour to a new point that corresponds to the thickness d . Joining such points, for the same value of film thickness d , at different values of ϕ , generates the constant-thickness contour, Fig. 6. The points on the ZTC at $\phi = 0^\circ$ and $\phi = 90^\circ$, which coincide with $\rho = -1$ and $\rho = +1$, respectively, stay the same for any value of d .

Figure 7 shows the $d = 1.5 \mu\text{m}$ constant-thickness contour of the ellipsometric function ρ in the complex ρ plane for the Si-SiO₂ system at $\lambda = 6328 \text{ \AA}$. This contour is traversed as the angle of incidence ϕ is increased starting from the point N ($\rho = -1$) when $\phi = 0^\circ$ (normal incidence) and ending at the point G ($\rho = +1$) when $\phi = 90^\circ$ (grazing incidence). The spiralling behavior near N shown by the constant-thickness contour of Fig. 7 is shared by other such contours for thicknesses comparable to or greater than λ . This spiralling can be attributed to the high density of the CAIC's near N (see Fig. 4) and to the fact that the thickness period D_ϕ of the CAIC is shortest (hence the rate of rotation is maximum) near $\phi = 0^\circ$ (see Fig. 3).

The angles ψ and Δ associated with the ellipsometric function $\rho = \tan\psi e^{j\Delta}$ [Eq. (4)] are plotted in Figs. 8 and 9 versus the angle of incidence ϕ as we move along the $1.5 \mu\text{m}$ constant-thickness contour of Fig. 7. Several significant points are marked on the CTC of Fig. 7 and on the ψ and Δ curves in Figs. 8 and 9, respectively. With the exception of N and G , these significant points are grouped as follows:

(i) The intersection points R_1, R_2, \dots of the CTC with the real axis of the complex ρ plane, which occur at angles of incidence $\phi_{r1}, \phi_{r2}, \dots$: The intersection R_i of the

CTC with the real axis is to the left or to the right of the origin if $\Delta = \pi$ or 0 , respectively. All intersections $R_1, R_2,$ and R_3 for the $d = 1.5 \mu\text{m}$ CTC shown in Fig. 7 correspond to $\Delta = \pi$ and occur at angles of incidence $\phi_{r1} = 30.13^\circ, \phi_{r2} = 46.75^\circ,$ and $\phi_{r3} = 62.44^\circ$, respectively. Such points appear in Fig. 9 as the intersections of the $\Delta - \phi$ curve with the $\Delta = \pi$ line. When $\Delta = 0$ or π , incident light that is linearly polarized at any azimuth relative to the plane of incidence is linearly polarized after it is reflected from the film-coated substrate. This suggests a new polarizer-surface-analyzer (PSA) null-ellipsometer arrangement without a compensator that can be used to characterize film-substrate systems for which the film thickness exceeds a certain minimum value so that one or more intersections of the CTC with the real axis become available. This minimum thickness, for the same system, depends on the wavelength; the smaller the wavelength used, the smaller the minimum thickness. Three such intersections are obtained at an oxide thickness of $1.5 \mu\text{m}$ in the case of the Si-SiO₂ system at 6328 \AA , Fig. 7. The nulling scheme would involve setting either the polarizer P or the analyzer A at a fixed azimuth and adjusting the other element (A or P , respectively), together with the angle of incidence ϕ , for null. The null condition can be obtained at as many angles of incidence ϕ_{rk} as there are intersections R_k of the CTC with the real axis, where $k = 1, 2, \dots$. Experimental measurements using this PSA null-ellipsometer arrangement were carried out on Si-SiO₂ system at a wavelength of 6328 \AA for different film thicknesses. The results obtained were quite close to the calculated values using the nominal film thickness and the published data for the optical constants³ of Si and SiO₂. Details of this novel method of null ellipsometry will be considered elsewhere.

(ii) The intersections I_1, I_2, \dots of the CTC with the imaginary axis of the complex ρ plane, which occur at angles of incidence $\phi_{i1}, \phi_{i2}, \dots$: At such points, $\Delta = \pi/2$ or $3\pi/2$, dependent on whether the intersection I is above or below the origin, respectively. When $\Delta = \pi/2$ or $3\pi/2$, the major and minor axes of the ellipse of polarization of the reflected light, when the incident light is linearly polarized at an arbitrary azimuth, are

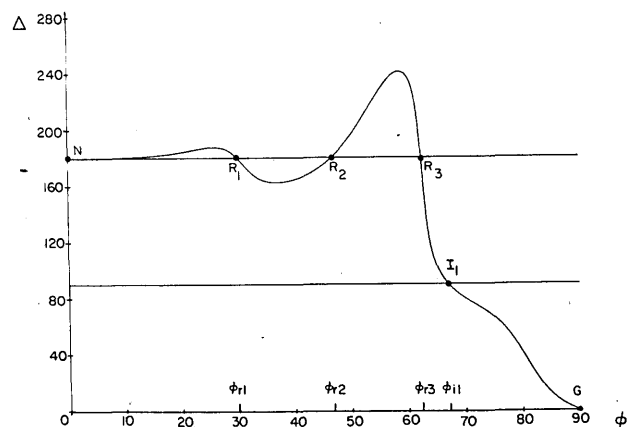


FIG. 9. The angle Δ as a function of the angle of incidence ϕ for Si-SiO₂ system at $\lambda = 6328 \text{ \AA}$ and film thickness $d = 1.5 \mu\text{m}$. Both Δ and ϕ are in degrees.

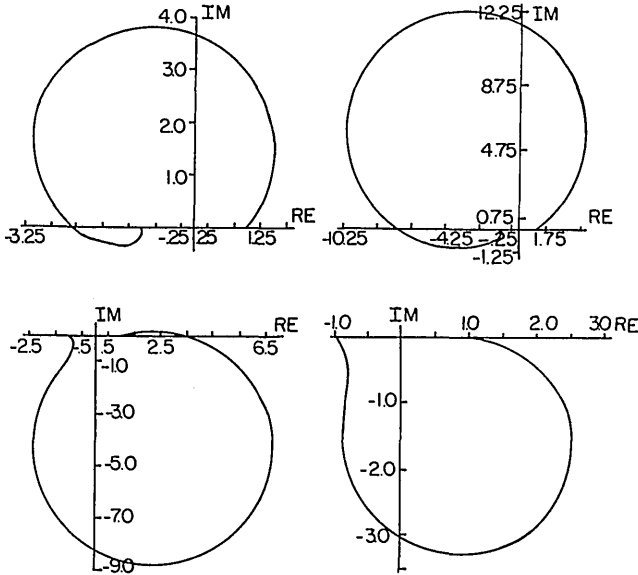


FIG. 10. A sequence of constant-thickness contours (CTC's) in the complex ρ plane for the Si-SiO₂ system at $\lambda = 6328 \text{ \AA}$ for different film thicknesses. Upper left: $d = 0.21\lambda$; upper right: $d = 0.22\lambda$; lower left: $d = 0.23\lambda$; and lower right: $d = 0.24\lambda$.

aligned parallel and perpendicular to the plane of incidence. The angles of incidence $\phi_{i1}, \phi_{i2}, \dots$ may be called the principal angles⁶ of incidence for the film-substrate system. For the $d = 1.5 \mu\text{m}$ CTC of Fig. 7, only one principal angle is available $\phi_{i1} = 67.19^\circ$. The I intersections appear in Fig. 9 as the intersections of the Δ -vs- ϕ curve with the $\Delta = \pi/2$ line.

(iii) The intersection points U_1, U_2, \dots of the CTC with the unit circle U of the complex ρ plane: At such intersections, we have $\tan\psi = 1$; hence $\psi = 45^\circ$. These points are shown in Fig. 8 as the intersections of the ψ -vs- ϕ curve with the $\psi = 45^\circ$ line. When $\tan\psi = 1$, we have $|R_p| = |R_s|$ and $\rho = e^{j\Delta}$ [see Eqs. (3) and (4)], and the film-substrate system acts as a reflection retarder. Such a retarder exhibits isotropic absorption because the absolute reflectances $\mathcal{R} = |R_p|^2 = |R_s|^2$ are necessarily less than 1. For the Si-SiO₂ system with $d = 1.5 \mu\text{m}$ at $\lambda = 6328 \text{ \AA}$, the angles of incidence at which exact operation as a retarder is achieved are $\phi_{u1} = 27.0^\circ$, $\phi_{u2} = 33.25^\circ$, $\phi_{u3} = 58.75^\circ$, and $\phi_{u4} = 66.75^\circ$. The associated retardations are $\Delta_{u1} = 187.62^\circ$, $\Delta_{u2} = 167.23^\circ$, $\Delta_{u3} = 240.9^\circ$, and $\Delta_{u4} = 92.03^\circ$, whereas the reflectances are $\mathcal{R}_{u1} = 0.105$, $\mathcal{R}_{u2} = 0.108$, $\mathcal{R}_{u3} = 0.155$, and $\mathcal{R}_{u4} = 0.208$, respectively. A more systematic approach to the design of retarders is discussed in Sec. III.

(iv) The points P_1 and P_2 where the minimum-radius and maximum-radius circles, centered on the origin, touch the CTC, respectively: These two concentric circles define an annular domain in which the CTC is confined. At P_1 and P_2 , $|\rho| = \tan\psi$ is minimum and maximum, respectively. These points indicate how a given film-substrate system comes close to operating as a p - or s -suppressing polarizer. When the minimum radius is zero, $\psi_{P1} = 0$, the CTC passes through the origin. At the corresponding angle of incidence ϕ_{P1} the film-substrate system acts exactly as a p -suppressing polar-

izer. On the other hand, when the maximum radius becomes infinitely large, $\psi_{P2} = 90^\circ$, the CTC passes through the point at infinity. At the corresponding angle of incidence ϕ_{P2} , the film-substrate system acts exactly as an s -suppressing polarizer. The basic design of such elements will also be discussed in Sec. III.

Figures 10 and 11 show two sequences of constant-thickness contours (CTC). As can be appreciated from these sequences, there is an infinite variety of such CTC's. Two CTC's may intersect one another, so that a given value of the ellipsometric function ρ can be realized at two different thicknesses at the same angle of incidence.⁷ This multiplicity is absent from the constant- ϕ contours, each of which is traced only once in the interval of film thickness $0 \leq d < D_\phi$, Eq. (14), where D_ϕ is given by Eq. (13) and shown in Fig. 3 for SiO₂ at $\lambda = 6328 \text{ \AA}$. By limiting the choice of thickness at each ϕ to the range specified by Eq. (14), i. e., by limiting ourselves to the area below the D_ϕ boundary curve in the (ϕ, d) space of Fig. 3, all values of the ellipsometric function ρ are generated only once. Notice that any (ϕ, d) point in Fig. 3 above the D_ϕ boundary curve can be brought vertically down (i. e., at the same ϕ) by subtraction of the appropriate multiple of the period D_ϕ . Recall that the ellipsometric function ρ [Eqs. (8) and (12)] is periodic in film thickness d , with an angle-of-incidence-dependent period D_ϕ .

III. DESIGN OF REFLECTION-TYPE FILM-SUBSTRATE OPTICAL DEVICES

We have seen that by varying the angle of incidence ϕ over the interval $0 \leq \phi \leq 90^\circ$, and varying the film thickness d at each angle ϕ over the thickness period $0 \leq d < D_\phi$ (Fig. 3), we cover the entirety of the complex ρ plane of the ellipsometric function ρ . In other words, a thickness value d and an angle of incidence ϕ can always be found that realize any given value of ρ , i. e., any given values of ψ and Δ . This assumes a film-substrate system with zero absorption in the film. Because

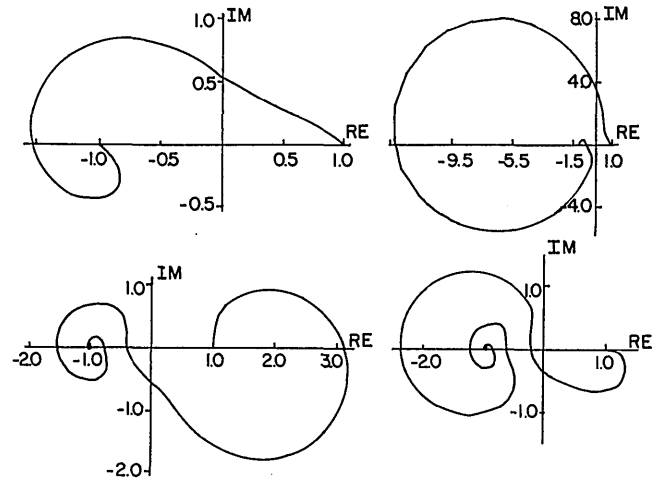


FIG. 11. A sequence of constant-thickness contours (CTC's) in the complex ρ plane for the Si-SiO₂ system at $\lambda = 6328 \text{ \AA}$ for different film thicknesses. Upper left: $d = \lambda$; upper right: $d = 2\lambda$; lower left: $d = 3\lambda$; and lower right: $d = 4\lambda$.

ρ determines completely the effect of reflection on the state of polarization of the incident light, determination of d and ϕ that lead to a prescribed value of ρ (or ψ and Δ) represents the main step in the design of film-substrate reflection optical devices.

A. Reflection polarizers

The ellipsometric function $\rho = R_p/R_s$ is a rational function of the complex exponential X , Eq. (8), that has one zero, $\rho = 0$, when

$$R_p = 0, \quad (18)$$

and one pole, $\rho = \infty$, when

$$R_s = 0. \quad (19)$$

Because ρ is the ratio of two quadratics, it has one additional pole and one additional zero plus those specified by Eqs. (18) and (19). They correspond to $R_p = \infty$ and $R_s = \infty$, respectively, and, hence, are of no physical meaning.

The condition $R_p = 0$ leads to a simple solution of Eq. (8) for X , namely [see Eqs. (1) and (6)]

$$\begin{aligned} r_{01p} + r_{12p}X &= 0, \\ X &= -(r_{01p}/r_{12p}). \end{aligned} \quad (20)$$

Because, for transparent films [Eqs. (12) and (13)],

$$|X| = 1, \quad (21)$$

a very simple procedure for the design of a film-substrate, p -suppressing, reflection polarizer becomes quite evident. The right-hand side of Eq. (20) is the ratio of the 0-1 and 1-2 interface Fresnel reflection coefficients for the p polarization, which are independent of film thickness and vary only with angle of incidence for a given film-substrate system. Thus, by plotting $|r_{01p}/r_{12p}| = |X|$ with the angle of incidence ϕ , the intersection of such a curve with the straight line $|X| = 1$ yields the polarizing angle of incidence at which suppression of the parallel polarization is possible by a film-substrate system. Figure 12 (upper left) shows a curve⁸ of $1 - |X|$ vs ϕ . Such a curve intersects the ϕ axis at the polarizing angle $\phi_p = 75.4401^\circ$. To determine the necessary film thickness for polarizer operation, let us write the complex Fresnel coefficients r_{01p} and r_{12p} as

$$r_{01p} = |r_{01p}| e^{j\delta_{01p}}, \quad r_{12p} = |r_{12p}| e^{j\delta_{12p}}, \quad (22)$$

where δ_{01p} and δ_{12p} are the interface phase jumps. By substituting r_{01p} and r_{12p} from Eqs. (22) and X from Eq. (12) into Eq. (20), we obtain

$$-e^{-j2\pi(d/D_{\phi_p})} = (|r_{01p}|/|r_{12p}|) e^{j(\delta_{01p} - \delta_{12p})}. \quad (23a)$$

At the p -polarizing angle ϕ_p , $|r_{01p}| = |r_{12p}|$, (this is how ϕ_p was found), so that Eq. (23a) becomes

$$-e^{-j2\pi(d_p/D_{\phi_p})} = e^{j(\delta_{01p} - \delta_{12p})_{\phi_p}}. \quad (23b)$$

D_{ϕ_p} and $(\delta_{01p} - \delta_{12p})_{\phi_p}$ are the values of D_{ϕ} and $(\delta_{01p} - \delta_{12p})$ evaluated at $\phi = \phi_p$. Equation (23b) can be immediately

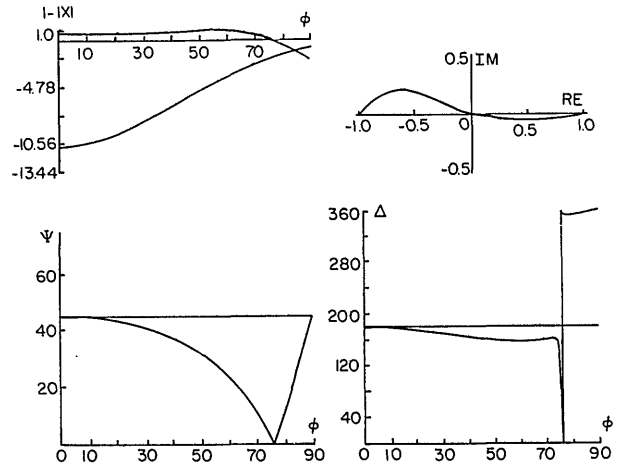


FIG. 12. This group of curves represent the design and performance of the p -suppressing polarizer for the Si-SiO₂ system at $\lambda = 6328 \text{ \AA}$. Upper left: The quantity $1 - |X|$, where X is the thickness complex-exponential function, plotted against the angle of incidence ϕ , where ϕ is in degrees. Upper right: The constant-thickness contour (CTC) for film thickness $d = 2891.73 \text{ \AA}$. Lower left: The angle ψ as a function of the angle of incidence ϕ for the same film thickness. Both ψ and ϕ are in degrees. Lower right: The angle Δ as a function of the angle of incidence ϕ for the same film thickness. Both Δ and ϕ are in degrees.

solved for the p -polarizing film thickness d_p ,

$$\begin{aligned} -2\pi(d_p/D_{\phi_p}) + 2\pi(m + \frac{1}{2}) &= (\delta_{01p} - \delta_{12p})_{\phi_p}, \\ (d_p/D_{\phi_p}) &= \frac{1}{2\pi}(\delta_{12p} - \delta_{01p})_{\phi_p} + (m + \frac{1}{2}), \end{aligned}$$

or

$$d_p = \frac{1}{2\pi}(\delta_{12p} - \delta_{01p})_{\phi_p} D_{\phi_p} + (m + \frac{1}{2}) D_{\phi_p}. \quad (24)$$

In Eq. (24), the appearance of the multiple mD_{ϕ_p} of the thickness period D_{ϕ_p} (m is an integer) is consistent with the fact that ρ is a periodic function of film thickness with a period equal to D_{ϕ_p} when $\phi = \phi_p$. For the Si-SiO₂ system, the least-polarizing thickness was found to be $d_p = 2891.73 \text{ \AA}$. The thickness period D_{ϕ_p} at $\phi = \phi_p$ was found to be 2894.61 \AA . Thus, the sequence of polarizing thicknesses in angstroms is 2891.73, 5786.34, 8680.95, ..., which are equispaced by the thickness period D_{ϕ_p} . The constant-thickness contour (CTC) at a polarizing thickness of 2891.73 \AA is shown in Fig. 12 (upper right). It passes through the origin ($\rho = 0$), as it should. The associated $\psi - \phi$ and $\Delta - \phi$ curves at that same thickness are shown in Fig. 12 (lower left and lower right, respectively). Notice that ψ drops to zero at the polarizing angle, Fig. 12 (lower left), and that Δ experiences a discontinuous jump of 2π at that angle, Fig. 12 (lower right). The calculated p and s reflectances, \mathcal{R}_{pp} and \mathcal{R}_{sp} , of this p -suppressing polarizer were found to be 0.23×10^{-4} and 0.76 , respectively.

The design of an s -suppressing polarizer follows exactly the same procedure that we outlined for the design of the p -suppressing polarizer. All we have to do is rewrite Eqs. (20)–(24) with an s subscript instead of a p

subscript. Our calculations for the Si-SiO₂ system at 6328 Å show that the *s*-polarizing angle $\phi_{sp} = 70.56^\circ$ and that the least-polarizing thickness $d_s = 1417.69$ Å. The thickness period D_{ϕ_s} at ϕ_s is equal to 2838.65 Å. Thus the infinite sequence of *s*-polarizing film thicknesses in angstroms is 1417.69, 4256.34, 7094.99, ... Figure 13 (upper right) shows the CTC at $d_s = 1417.69$ Å and Fig. 13 (lower left and lower right) give the associated $\psi - \phi$ and $\Delta - \phi$ curves. Note that the CTC passes through the point at infinity, Fig. 13 (upper right), that $\psi = 90^\circ$ at $\phi = \phi_s$, Fig. 13 (lower left), and that Δ experiences a discontinuous jump of π at ϕ_s , Fig. 13 (lower right). The calculated *p* and *s* reflectances of the above *s*-suppressing polarizer, R_{ps} and R_{ss} , are 0.28 and 0.19×10^{-11} , respectively.

The above approach to the design of reflection film-substrate polarizers is equivalent to that of Ruiz-Urbieta *et al.*⁹⁻¹¹ However, the analysis leading to the design equations is much simpler. The simplicity comes from working with the complex amplitude-reflection coefficients $R_{p,s}$ directly rather than the reflectances $R_{p,s} = |R_{p,s}|^2$ and the realization that for zero reflectance, $R_{p,s} = 0$, the complex amplitude-reflection coefficient $R_{p,s}$ must itself be zero.

B. Reflection retarders

To realize any value of the ellipsometric function ρ , we can generally solve Eq. (8) for X in terms of ρ

$$X = \frac{-(B - \rho E) \pm [(B - \rho E)^2 - 4(C - \rho F)(A - \rho D)]^{1/2}}{2(C - \rho F)}, \quad (25)$$

where A , B , C , D , E , and F are functions of the interface reflection coefficients r_{01p} , r_{01s} , r_{12p} , and r_{12s} only, Eqs. (10) and (11). To determine the angle of incidence ϕ at which a given value of ρ is realizable, we make use of the fact that $|X| = 1$ and that the right-hand side of Eq. (25) is a function of ϕ only. Thus, by plotting $1 - |X|$ vs ϕ , the intersection of the resulting curve with the ϕ axis gives the desired value of ϕ . Equation (25) predicts two branches for $1 - |X|$ corresponding to the two complex roots. Only one of them can intersect the ϕ axis because of the nonintersecting nature of the constant-angle-of-incidence contours (CAIC), Fig. 4. The required film thickness together with the above-determined angle of incidence lead to the specified value of ρ . Let α be the angle of the complex number on the right-hand side of Eq. (25). Then

$$-2\pi(d/D_\phi) + m2\pi = \alpha,$$

from which

$$d = -\frac{\alpha}{2\pi} D_\phi + mD_\phi, \quad (26)$$

where α and D_ϕ are evaluated at the previously determined ϕ .

The design of any retarder is a special case of the foregoing general scheme.¹² In this case

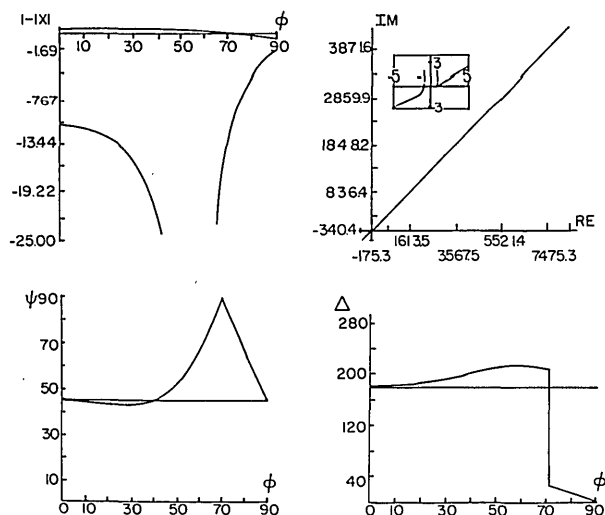


FIG. 13. This group of curves represent the design and performance of the *s*-suppressing polarizer for the Si-SiO₂ system at $\lambda = 6328$ Å. Upper left: The quantity $1 - |X|$, where X is the thickness complex-exponential function plotted against the angle of incidence ϕ , where ϕ is in degrees. Upper right: The constant-thickness contour (CTC) for film thickness $d_s = 1417.69$ Å. The part of the curve around zero is shown in the box on a different scale. Lower left: The angle ψ as a function of the angle of incidence ϕ for the same film thickness. Both ψ and ϕ are in degrees. Lower right: The angle Δ as a function of the angle of incidence ϕ for the same film thickness. Both Δ and ϕ are in degrees.

$$\rho = e^{j\Delta}, \quad (27)$$

where Δ is the desired retardation. For a quarter-wave retarder (QWR), $\Delta = \pi/2$ and $\rho = +j$. By substituting this value of ρ into Eq. (25), we calculated $1 - |X_1|$ and $1 - |X_2|$ vs ϕ for the Si-SiO₂ system at 6328 Å. The results are shown in Fig. 14 (upper left). Notice that only one branch $|X_1|$ intersects the ϕ axis. The angle of intersection $\phi_{QWR} = 67.29^\circ$. The smallest film thickness for operation as a quarter-wave retarder $d_{QWR} = 1056.29$ Å, is obtained from Eq. (26) where $m = 0$. The reflectances of this QWR are $R_{pQWR} = R_{sQWR} = 0.215$. Figure 14 (upper right) shows the CTC corresponding to d_{QWR} . Such a curve passes through the point $+j$ on the imaginary axis, as expected. Figure 14 (lower left) shows ψ vs ϕ when $d = d_{QWR}$, while Fig. 14 (lower right) shows Δ vs ϕ for the same thickness. Note that ψ stays quite close to the $\psi = +45^\circ$ line, leading to the very interesting conclusion that such a film-substrate system can operate as an angle-of-incidence tunable retarder. The tuning curve of such a retarder is Fig. 14 (lower right).

IV. INVERSION OF THE NONLINEAR EQUATIONS OF REFLECTION ELLIPSOMETRY

From the above, we have seen that for transparent films any value of the ellipsometric function ρ can be realized by solving Eq. (8) for X in terms of ρ , Eq. (25). The coefficients A , B , C , D , E , and F of Eq. (25) are functions of the angle of incidence ϕ and the optical

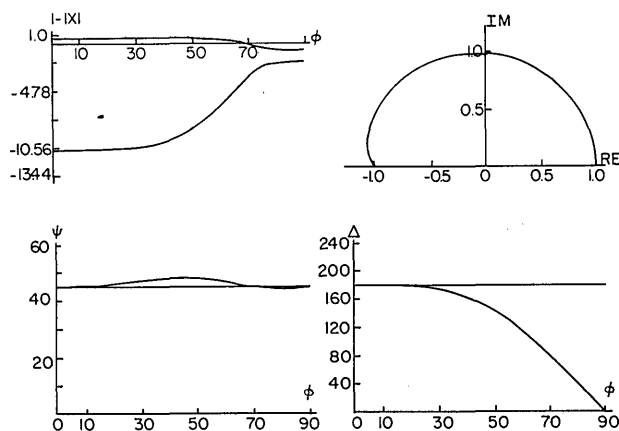


FIG. 14. This group of curves represent the design and performance of the quarter-wave-retarder for the Si-SiO₂ system at $\lambda = 6328 \text{ \AA}$. Upper left: The quantity $1 - |X|$, where X is the thickness complex-exponential function, plotted against the angle of incidence ϕ , where ϕ is in degrees. Upper right: The constant-thickness contour (CTC) at film thickness $d_{QWR} = 1056.29 \text{ \AA}$. Lower left: The angle ψ as a function of the angle of incidence ϕ for the same film thickness. Both ψ and ϕ are in degrees. Lower right: The angle Δ as a function of the angle of incidence ϕ for the same film thickness. Both Δ and ϕ are in degrees.

constants (refractive indices and extinction coefficients) of the ambient, film, and substrate only, but not of the film thickness d . Also, we found that X should satisfy the condition $|X| = 1$, Eq. (21). Therefore, if the angle of incidence ϕ , the wavelength λ , and the ellipsometric function ρ are known, the optical constants of the film and the substrate should satisfy the condition $|X| = 1$, Eq. (21), independently of the film thickness d . By reflection ellipsometry, we measure the ellipsometric function ρ at a given angle of incidence ϕ and wavelength λ . The number of independent measurements necessary for the inversion procedure depends on the number of unknowns to be determined. We need one measurement for each pair of unknowns. To carry out the inversion process, we write the required equations, one from each measurement, in the form of $|X| = 1$, where X is given by Eq. (25). The required independent measurements can be made, for example, at multiple angles of incidence. The numerical-inversion procedure is to iterate on the optical constants of both the film and the substrate until the condition $|X| = 1$, where X is given by Eq. (25), is satisfied for all such equations. Substituting the optical constants thus obtained into Eq. (26), we obtain the film thickness.¹³

The foregoing outlines a unique method of separating the determination of the optical constants of the film and substrate from that of the film thickness. As a simple special case, a simulation study was carried out to determine the film refractive index N_1 and its thickness for Si-SiO₂ system at a wavelength of 6328 \AA . The results confirmed the method outlined. An error of 0.1° in the angle of incidence ϕ produces an error of 0.001 in the determination of the film refractive index N_1 of 1.46 and an error of 50 \AA in the determination of an assumed

film thickness of 31640 \AA .

Reinberg¹⁴ arrived at a method equivalent to ours for the special case of solving for the refractive index N_1 and thickness d of a nonabsorbing film. However, our method can provide the solution for all of the parameters of a filmed substrate, that is, the refractive index N_1 of a nonabsorbing film and n_2 and k_2 , the refractive index and extinction coefficient of the substrate in addition to the film thickness d .

V. EFFECT OF FILM ABSORPTION

We close with a brief discussion of the effect of film absorption, which is generally applicable to either the design of the reflection-type optical devices or to the inversion procedure that we have discussed previously in Sec. III and IV, respectively. The concepts remain the same as for transparent films, but the condition of Eq. (21), $|X| = 1$, is no longer satisfied. When the film is absorbing, the complex exponential function X , Eqs. (9), (12), and (13), traces a convergent logarithmic spiral in the complex X plane, instead of the unit circle in the case of transparent films. Note that the exponential function of Eq. (12) contains a damping term in addition to the periodic term, because the film refractive index N_1 is a complex quantity. Because of this damping term, the procedure to find the angle of incidence ϕ and the film thickness d that realize a given value of the ellipsometric function ρ is changed.

Equation (25) continues to provide the solution for X in terms of the ellipsometric function to be realized and the interface reflection coefficients r_{01p} , r_{01s} , r_{12p} , and r_{12s} independent of the film thickness d . By taking the logarithms of both sides of Eq. (12), we obtain

$$\ln(X) = -j2\pi(d/D_0), \quad (28)$$

where X is given by Eq. (25). From Eqs. (28) and (13), we get

$$d = j(\lambda/4\pi)(N_1^2 - \sin^2\phi)^{-1/2} \ln(X) + \frac{1}{2}m\lambda(N_1^2 - \sin^2\phi)^{-1/2}, \quad (29)$$

where the second term has been added because X and $Xe^{j2\pi\sigma}$ are indistinguishable, m being a positive or negative integer.

Equation (29) is the basis of a procedure for obtaining the angle of incidence ϕ and the film thickness d that realize the ellipsometric function ρ . For a given film-substrate system, at a given wavelength, the right-hand side of Eq. (29) is a complex function of the angle of incidence only. The left-hand side is always real and equals the film thickness. Thus, to get the solution of Eq. (29), the angle of incidence ϕ should satisfy the condition that the right-hand side of this equation is real. If we plot the right-hand side of the equation in the complex plane as a function of the angle of incidence ϕ , the intersection of the resulting curve with the real axis gives the value of the film thickness d . The angle of incidence at which the intersection occurs gives the required angle of incidence. Note that we have to plot

the right-hand side of Eq. (29) for each value of m ($m=0, \pm 1, \pm 2, \dots$) leading to a number of possible solution sets for the film thickness d and the angle of incidence ϕ . As the film absorption increases, the number of discrete solution sets (ϕ_m, d_m), $m=0, \pm 1, \dots$ that realize the required ρ are expected to become smaller until the required ρ is realized at only one thickness and one angle of incidence, or not at all.

To determine the optical constants of both the film and the substrate ($n_1, k_1; n_2, k_2$) and the film thickness d from multiple ellipsometric measurements, an adequate set of independent equations of the form of Eq. (29), to be obtained from the multiple measurements, is solved by iterating on the optical constants in a manner analogous to the procedure outlined in Sec. IV for nonabsorbing films.

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¹*Ellipsometry in the Measurement of Surfaces and Thin Films*, edited by E. Passaglia, R. Stromberg, and J. Kruger, Natl. Bur. Std. (U.S.) Misc. Pub. 1, No. 256 (U. S. Government Printing Office, Washington, D. C., 1961).

²*Proceedings of the Symposium on Recent Developments in Ellipsometry*, edited by N. M. Bashara, A. B. Buckman, and A. C. Hall (North-Holland, Amsterdam, 1968).

³*Ellipsometric Tables of the Si-SiO₂ System for Mercury and He-Ne Laser Spectral Lines*, edited by G. Gergely (Akademiai Kiado, Budapest, 1971).

⁴The significance of this was appreciated by A. B. Winterbottom, *Optical Studies of Metal Surfaces*, Kgl. Norske Vidensk. Selsk. Skrift., Vol. 1 (F. Bruns, Trondheim, 1955).

⁵Such contours are also called the polar curves. See the paper by P. C. S. Hayfield, Ref. 1, pp. 157ff.

⁶The principal angle is defined for a bare substrate as that angle at which $\Delta = \pi/2$.

⁷These thicknesses are spaced by an integral multiple of the thickness period D_ϕ evaluated at the common angle of incidence ϕ .

⁸Two branches are shown in Fig. 12 (upper left). The lower branch is generated from the condition that $R_s = \infty$ which has no physical existence but leads to $\rho=0$. In this case, $x = -1/\tau_{01s}\tau_{12s}$, from which the lower branch is calculated. Both the upper and lower branches are predicted by the general design equation, Eq. (25), in which, for the present case of a p -suppressing reflection polarizer, ρ is set equal to zero.

⁹M. Ruiz-Urbieta and E. M. Sparrow, *J. Opt. Soc. Am.* 62, 1188 (1972).

¹⁰M. Ruiz-Urbieta and E. M. Sparrow, *J. Opt. Soc. Am.* 63, 194 (1973).

¹¹M. Ruiz-Urbieta, E. M. Sparrow, and G. W. Goldman, *Appl. Opt.* 12, 590 (1973).

¹²So also is the design of reflection polarizers. For the p -suppressing and s -suppressing reflection polarizers, the values of ρ to be substituted in the right-hand side of Eq. (25) are 0 and ∞ , respectively.

¹³This film thickness is the least one; to get the correct film thickness the appropriate multiple of D_ϕ should be added.

¹⁴A. R. Reinberg, *Appl. Opt.* 11, 1273 (1972). We want to thank a reviewer for calling this reference to our attention.