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Single-pass polarizer–surface-analyzer null ellipsometry (PSA-NE) can be used to characterize film–substrate systems, provided that the film thickness lies within one of a set of permissible-thickness bands (PTB). For a transparent film on a transparent or absorbing substrate, the PTB structure consists of a small number of finite-bandwidth bands followed by a continuum band that extends from a film thickness of about half the wavelength of light to infinity. We show that this band structure is a direct consequence of the periodicity of the ellipsometric function ρ (the ratio R_p/R_s of the complex amplitude-reflection coefficients for the p and s polarizations) with film thickness. The PTB for the SiO_2-Si film–substrate system at He–Ne laser and mercury spectral lines are calculated. The angles of incidence for PSA-NE on a film–substrate system with known film thickness are easily predicted with the help of a graphical construction in the angle of incidence-vs-thickness ϕd plane. PSA-NE is generally applicable to the determination of both film thickness and optical properties of a film–substrate system. The procedure for its application to the special, but important, case of film-thickness measurement alone, when the optical properties are known, is given and is checked experimentally by the determination of the oxide-film thickness on Si wafers. In an automated form, PSA-NE can be a serious competitor for interferometric reflectance methods.

Index Headings: Ellipsometry; Polarization; Reflection; Films; Silicon.

When light is obliquely reflected from an optically isotropic surface S, its two component waves that are linearly polarized with their electric fields vibrating parallel (p) and perpendicular (s) to the plane of incidence experience different phase shifts, δ_p and δ_s, respectively. The difference between these phase shifts, $\Delta = \delta_p - \delta_s$, is generally neither 0 nor π for angles of incidence $0 < \phi < 90°$, so that incident linearly polarized light of arbitrary azimuth becomes elliptically polarized upon reflection. Consequently, light cannot be extinguished or nulled when the reflector S is placed between a linear polarizer P and analyzer A, Fig. 1, unless the transmission axes of the polarizer and analyzer are oriented one parallel and the other perpendicular to the plane of incidence. To obtain nontrivial nulls by P and A, a compensator C needs to be inserted either before or after S, to eliminate (compensate) the reflection phase difference Δ. This is the basis of two commonly used (PCSA and PSCA) null-ellipsometer arrangements.[1]

It is obvious that if $\Delta = 0$ or π at oblique incidence, no compensator would be needed and PSA null ellipsometry (PSA-NE) can be used. The condition $\Delta = 0$ or π is satisfied by a film-free homogeneous dielectric substrate, at all angles of incidence. In the presence of absorption or overlay films, this is no longer true. To be able to do null ellipsometry without a compensator on surfaces with $\Delta \neq 0$ or π, O'Bryan developed an ingenious method.[2] O'Bryan exploited the fact that Δ can be made equal to $\pi/2$ by adjusting the angle of incidence so that it equals the principal angle, and folded the reflected beam back on itself by a perpendicular mirror so that two reflections gave $\Delta = \pi$. By control of the azimuth of one polarizer and the angle of incidence, the retroreflected beam could be extinguished. First described in 1936, this elegant ellipsometer, which employs only one polarizing optical component, had apparently been forgotten and has recently been rediscovered.[3]

In this paper, we show that single-pass PSA-NE can be used to characterize film–substrate systems, pro-

vided that the film thickness lies within certain permissible-thickness bands (PTB). This possibility has been recently discovered[4]; here we elaborate on it. For the purpose of illustration, we take the SiO_2-Si system at $\lambda = 6328$ Å as an example in some parts of the subsequent analysis. However, the discussion is valid for any transparent film on an absorbing substrate at any wavelength. Also, our results can be generalized to apply to absorbing films, but this will not be dealt with here.

I. BEHAVIOR OF THE ELLIPSOMETRIC ANGLE Δ AS A FUNCTION OF THE ANGLE OF INCIDENCE ϕ FOR A FILM-SUBSTRATE SYSTEM

For a bare substrate (Si) the reflection phase difference Δ is a monotonically decreasing function of the angle of incidence ϕ, falling from π at $\phi = 0$ (normal incidence) to 0 at $\phi = 90°$ (grazing incidence), Fig. 2-left (continuous curve). The presence of a very-thin film (SiO_2; $d = 20$ Å) does not change the monotonic character of the Δ-vs-ϕ curve, Fig. 2-left (dashed curve). However, as the thickness d of the transparent film (SiO_2) is increased beyond a certain minimum value, the monotonic nature of the Δ-vs-ϕ curve ceases and gives way to an oscillatory (non-monotonic) behavior with one or more intersections of the curve with the $\Delta = \pi$ or 2π (0)
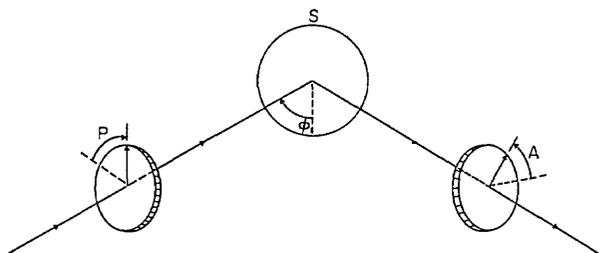

FIG. 1. Polarizer (P)–surface (S)–analyzer (A) ellipsometer. In the nulling mode, one of the azimuths P or A is fixed and the other, together with the angle of incidence ϕ, are adjusted to extinguish the light transmitted by the PSA optical train.
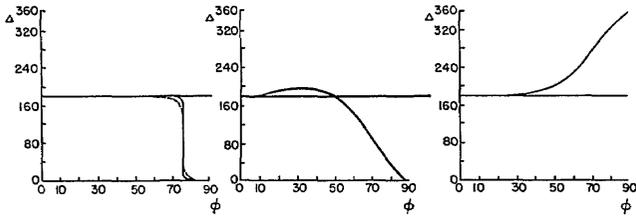
FIG. 2. *Left.* Monotonic Δ-vs-ϕ curves for a bare substrate (Si; continuous line) and a substrate (Si) covered by a very thin film (SiO$_2$; 20 Å; dashed line) (at $\lambda = 6328$ Å). *Middle.* Oscillatory Δ-vs-ϕ curve for a film–substrate (SiO$_2$-Si) system with film thickness ($d = 1200$ Å) in a PTB (at $\lambda = 6328$ Å). *Right.* Monotonic Δ-vs-ϕ curve for a film–substrate (SiO$_2$-Si) system with a film thickness ($d = 2167$ Å) that corresponds to a band edge (at $\lambda = 6328$ Å).

lines, Fig. 2-middle ($d = 1200$ Å).

In the following section, we arrive at the very interesting conclusion that the Δ-vs-ϕ curve is oscillatory and has intersections with the $\Delta = \pi$ or 2π (0) lines when the film thickness d lies within any one of a set of PTB[5]:

$$d_{il} < d < d_{iu}, \quad i = 1, 2, 3, \ldots, L,$$

where d_{il} and d_{iu} represent the lower and upper limits of the ith band, respectively. Furthermore, we find that the upper thickness limit of the last (upper-most) thickness band, d_{Lu}, is infinity ($d_{Lu} = \infty$) so that the top band is actually a continuum. A film-thickness value in the finite bands,

$$d_{il} < d < d_{iu}, \quad i = 1, 2, 3, \ldots, L-1, \tag{1}$$

and in the infinite continuum band,

$$d > d_{Ll}, \tag{2}$$

leads to an oscillatory Δ-vs-ϕ curve with one or more intersections with the $\Delta = \pi$ or $\Delta = 0$ (2π) lines at oblique angles of incidence ϕ_k ($k = 1, 2, \ldots$), $0 < \phi_k < 90°$. In these thickness ranges [Eqs. (1) and (2)], the film-substrate system can be characterized by PSA–NE, without a compensator.

When the film thickness corresponds to a band edge, a monotonic Δ-vs-ϕ curve with zero initial slope at $\phi = 0$, $\partial \Delta / \partial \phi = 0$, is obtained. This situation is represented in Fig. 2-right ($d = d_{2l} = 2167$ Å).

II. PTB FOR PSA-NE ON A FILM–SUBSTRATE SYSTEM

Now that we have stated the basic fact that governs the use of PSA-NE for a film–substrate system, namely the existence of PTB for which such operation is possible, we explain in this section how this result came about, and we determine the PTB for the SiO$_2$-Si system at $\lambda = 6328$ Å.

Origin of the PTB

The quantity measured by an ellipsometer is the ratio

$$\rho = R_p / R_s \tag{3}$$

of the complex amplitude-reflection coefficients R_p and R_s of an optically isotropic surface for the parallel (p) and perpendicular (s) polarizations. In Ref. 4, we investigated the behavior of the ellipsometric function ρ

for a film–substrate system as the angle of incidence ϕ and the film thickness d are permitted to scan their entire ranges $0 \leq \phi \leq 90°$, and $0 \leq d < \infty$, respectively. Figure 3 shows the complex plane of the ellipsometric function ρ (left), and the real plane of its two arguments ϕ and d (right). At a fixed angle of incidence ϕ, if the thickness d of a transparent film is increased from zero, the point ρ moves, in the complex ρ plane, from B on the zero-thickness contour (ZTC) which represents the bare substrate, along a closed constant-angle-of-incidence contour[4] (CAIC). The real axis is crossed first at H, where $d = d_H$, then at L, where $d = d_L$. Further increase of the film thickness d beyond d_L brings the point ρ back to its initial position B when $d = D_\phi$, which is the angle-of-incidence-dependent film-thickness period[6] of the function $\rho(\phi, d)$. Because ρ is a real number at both H and L, linearly polarized light of arbitrary azimuth, incident at a fixed angle of incidence ϕ on a substrate covered by a transparent film, is reflected linearly polarized at two discrete film thicknesses d_H and d_L, where

$$0 < d_H < d_L < D_\phi . \tag{4}$$

Because ρ is a periodic function of d, with period D_ϕ, we can generalize by saying that the reflected light becomes linearly polarized twice, at $d = d_H + m D_\phi$ and $d = d_L + m D_\phi$, as the film thickness d scans each period

$$m D_\phi < d < (m+1) D_\phi, \quad m = 0, 1, 2, 3, \ldots . \tag{5}$$

If we now allow ϕ to scan its range from 0 to 90°, the point H moves along the negative real axis of the complex ρ plane (Fig. 3-left) from N ($\rho = -1$, normal incidence, $\phi = 0$) to the point at infinity S ($\rho = \mp\infty$, s suppression,[7] $\phi = \phi_s$) and back along the positive real axis to G ($\rho = +1$, grazing incidence, $\phi = 90°$). The corresponding (image) point (ϕ, d_H) in the ϕd plane generates a curve of monotonically increasing thickness between $\phi = 0$ and $\phi = 90°$ (Fig. 3-right). Meanwhile, the point L moves along the segment of the real axis between N and G that passes through P ($\rho = 0$, p suppression,[7] $\phi = \phi_p$), Fig. 3-left, as ϕ increases from 0 to 90°. The image point (ϕ, d_L), Fig. 3-right, generates a second curve of monotonically increasing thickness between
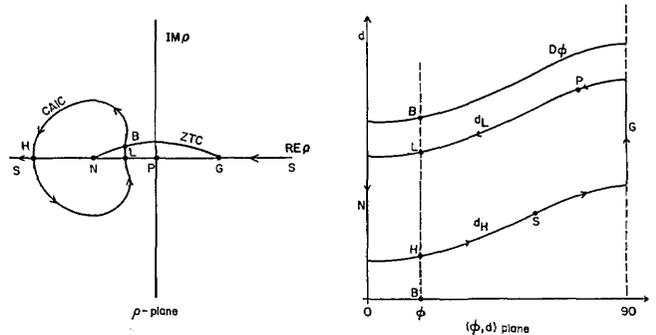

FIG. 3. Mapping between the complex plane of the ellipsometric function ρ (left) and the plane of its two real arguments; the angle of incidence ϕ and the film thickness d (right). Points that are the images of one another are identified by the same letter. The real axis of the complex ρ plane is mapped into a closed contour in the ϕd plane, NSGPN. The origin of the PTB for PSA-NE is explained with the help of this figure.

$\phi = 0$ and $\phi = 90°$. If we write

$$\rho = \tan\psi\, e^{j\Delta}, \tag{6}$$

then for H,

$$|\rho_H| > 1, \quad 45° < \psi_H \leq 90°, \tag{7a}$$

and for L,

$$|\rho_L| < 1, \quad 0 \leq \psi_L < 45°, \tag{7b}$$

and $\psi = 45°$ at the limiting points N and G. Consequently, the curves d_H and d_L in the reduced-thickness zone (RTZ)

$$0 \leq d < D_\phi, \quad 0 \leq \phi \leq 90°, \tag{8}$$

of the ϕd plane correspond to high-psi ($45° < \psi \leq 90°$) and low-psi ($0 \leq \psi < 45°$) branches (HPB and LPB), respectively. (This explains the choice of the letters H and L to identify these two branches.) The HPB d_H is divided into two segments by the point S (which represents the s-suppressing polarizer): on one segment, NS, $\Delta = \pi$; and on the other, SG, $\Delta = 0$. Likewise, the LPB d_L is divided into two segments by the point P (which represents the p-suppressing polarizer): on one segment, NP, $\Delta = \pi$; and on the other, PG, $\Delta = 0$. The entire real axis of the ρ plane, $NSGPN$ (Fig. 3-left), is mapped into a closed contour in the ϕd plane (Fig. 3-right) that consists of the two branches d_H, d_L and the vertical line segments between these two branches at $\phi = 0$ and $\phi = 90°$. [The two lines $\phi = 0$ and $\phi = 90°$ in the ϕd plane are mapped onto the single points $N(\rho = -1)$ and $G(\rho = +1)$, respectively, in the ρ plane.]

Let d_{H0} and d_{H90} be the lower and upper thickness limits of the HPB, d_H, at $\phi = 0$ and $90°$, respectively; and let d_{L0} and d_{L90} be the corresponding thickness limits for the LPB, d_L. Although the thickness gap,

$$\Delta d_G = d_L - d_H, \tag{9}$$

between the LPB and HPB is always positive for all angles of incidence, i.e.,

$$\Delta d_G > 0, \quad 0 \leq \phi \leq 90°, \tag{10}$$

two cases, Fig. 4, can be distinguished:

$$\text{case 1,} \quad d_{L0} > d_{H90}, \tag{11a}$$

$$\text{case 2,} \quad d_{L0} < d_{H90}. \tag{11b}$$

In case 1, Fig. 4-left, the two thickness ranges

$$d_{H0} \leq d_H \leq d_{H90}, \quad d_{L0} \leq d_L \leq d_{L90}, \tag{12}$$

are nonoverlapping, and the two branches d_H and d_L define two separate PTB, to be called the two base bands [because these bands exist in the RTZ, Eqs. (8)]. These represent the first two bands (1 and 2) in the band structure referred to in Sec. I. In terms of the general notation of Sec. I, we have

$$d_{1l} = d_{H0}, \quad d_{1u} = d_{H90};$$

$$d_{2l} = d_{L0}, \quad d_{2u} = d_{L90}. \tag{13a}$$

In case 2, Fig. 4-right, the two thickness ranges of Eqs. (12) are overlapping and merge into one base band whose lower and upper limits are given by

$$d_{1l} = d_{H0}, \quad d_{1u} = d_{L90}. \tag{13b}$$

Whether case 1 or case 2 is applicable depends on the particular film–substrate system and wavelength under consideration.

Once the base bands have been established, it is an easy matter to compute the band structure of all PTB for PSA-NE on a given film–substrate system at a given wavelength. Because the ellipsometric function ρ is periodic in the film thickness d, the base bands can be translated vertically upwards along the thickness axis by adding the same multiple of the film-thickness period D_0 (at $\phi = 0$) and D_{90} (at $\phi = 90°$) to the lower and upper limits of a base band, respectively.[8] Thus the thickness limits of a band obtained from translating base band 1 by adding m thickness periods are[9]

$$d_l^{1m} = d_{1l} + mD_0, \quad d_u^{1m} = d_{1u} + mD_{90}. \tag{14a}$$

Similarly, the thickness limits of a band obtained from translating base band 2 (if present) by n thickness periods are

$$d_l^{2n} = d_{2l} + nD_0, \quad d_u^{2n} = d_{2u} + nD_{90}. \tag{14b}$$

The translated bands, Eqs. (14), do not necessarily constitute separate bands by themselves because their thickness ranges may overlap. The true structure and thickness limits of the higher bands will depend on this overlapping of the translated bands. Also, because $D_{90} > D_0$, it will take only a few translations m_{max} and n_{max}, after which all translated bands will be parts of a continuum higher band extending to infinity. Because the procedure of synthesizing the band structure from the base bands is simple, we will not attempt to derive general equations that give the thickness limits of the true higher bands.

It is important to realize that the foregoing discussion of the PTB is based on the periodicity of the ellipsometric function ρ with the film thickness d and on the corollary fact that the CAIC is closed and encloses either $\rho = -1$ or $\rho = +1$ on the real axis of the complex ρ plane. The discussion is applicable to any system that consists of a substrate covered by a transparent film, provided that both the substrate and film are homogeneous and optically isotropic. The medium of incidence is also assumed to be transparent, homogeneous, and optically isotropic.

For a given ambient-film-substrate system at a given wavelength, the HPB and LPB can be exactly calculated by use of the method given in Ref. 4. Specifically, the
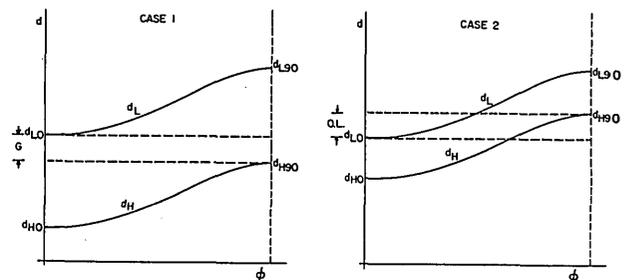

FIG. 4. The cases of (1) separate (left), and (2) overlapping (right) permissible base bands. In case (2) (right), the two base bands merge together to form one permissible band.

angle of incidence ϕ and the film thickness d that realize any given value of ρ can be obtained by Eqs. (25) and (26) of Ref. 4 according to the procedure outlined in the paragraph that contains those two equations. Once the HPB and LPB have been computed, the entire structure of the PTB can be easily determined, as explained in the foregoing.

HPB and LPB and the PTB for PSA-NE on the SiO$_2$-Si system at $\lambda = 6328$ Å

We have calculated the HPB and LPB and the PTB for PSA-NE on the SiO$_2$-Si system at $\lambda = 6328$ Å. The refractive indices of SiO$_2$ and Si at $\lambda = 6328$ Å are taken as 1.46 and 3.85-j0.02, respectively.[10] The ambient (medium of incidence) is assumed to be air.

Values of ρ that correspond to points in the different regions of the real axis marked in Fig. 3-left were calculated from Eq. (6), with ψ taken between 0 and 90° in steps of 5° and $\Delta = 0$ or π. These values were subsequently substituted into Eq. (25) of Ref. 3 and the corresponding angle of incidence ϕ and least thickness d were obtained as explained in that reference. The results are summarized in Tables I and II, for the HPB and LPB, respectively. Columns 1 and 2 of Tables I and II give the assumed values of Δ and ψ, and columns 3 and 4 give the angle of incidence ϕ and the least film thickness d (equal to d_H or d_L). For completeness, we list the thickness period D_ϕ, and the p and s reflectances $\mathfrak{R}_p$ and $\mathfrak{R}_s$ in columns 5, 6, and 7, respectively, of Tables I and II.

Figure 5 shows a plot of the two branches (ϕ, d_H) and (ϕ, d_L) in the ϕd plane. The lower and upper thickness limits of the HPB and LPB are $d_{H0} = 1083$, and $d_{H90} = 1487$ Å; and $d_{L0} = 2164$, and $d_{L90} = 2973$ Å. Note that $d_{L0} > d_{H90}$ [Eq. (11a)], so that the thickness ranges of the HPB and LPB are nonoverlapping and define two separate base bands. By the addition of multi-

TABLE I. Angle of incidence ϕ and reduced film thickness d for a SiO$_2$-Si film–substrate system at $\lambda = 6328$ Å that lead to $\Delta = 0$ or π (thus allowing PSA-NE) for different values of ψ in the range $45° < \psi \leq 90°$ (HPB). D_ϕ is the film-thickness period and $\mathfrak{R}_p$ and $\mathfrak{R}_s$ are the p and s reflectances.

Δ (deg.)	ψ (deg.)	ϕ (deg.)	d_H (Å)	D_ϕ (Å)	$\mathfrak{R}_p$	$\mathfrak{R}_s$
	45[a]	2.362	1083.2	2168.0	0.0826	0.0825
	50	37.860	1193.2	2388.4	0.0975	0.0686
	55	46.764	1249.2	2500.7	0.1136	0.0557
	60	52.414	1288.8	2580.3	0.1310	0.0437
180	65	56.660	1320.0	2642.5	0.1500	0.0326
	70	60.129	1345.4	2693.7	0.1709	0.0226
	75	63.117	1367.2	2737.3	0.1939	0.0139
	80	65.789	1386.1	2775.3	0.2197	0.0068
	85	68.247	1402.8	2808.8	0.2487	0.0019
	90	70.560	1417.7	2838.6	0.2817	4×10^{-12}
	85	72.778	1431.0	2865.4	0.3197	0.0024
	80	74.937	1443.0	2889.4	0.3637	0.0113
	75	77.066	1453.6	2910.6	0.4152	0.0298
0	70	79.187	1462.8	2929.1	0.4760	0.0631
	65	81.315	1470.6	2944.8	0.5481	0.1192
	60	83.460	1476.9	2957.4	0.6339	0.2113
	55	85.625	1481.5	2966.7	0.7361	0.3609
	50	87.807	1484.4	2972.4	0.8573	0.6036
	45[a]	89.996	1485.3	2974.3	0.9986	0.9955

[a]The value of ψ actually used was 45.01°.

TABLE II. Same as in Table I but for ψ in the range $0 \leq \psi < 45°$. (LPB).

Δ (deg.)	ψ (deg.)	ϕ (deg.)	d_L (Å)	D_ϕ (Å)	$\mathfrak{R}_p$	$\mathfrak{R}_s$
	45[a]	1.487	2164.7	2167.5	0.3452	0.3454
	40	32.112	2324.0	2326.8	0.2852	0.4051
	35	43.914	2459.9	2462.8	0.2270	0.4629
	30	52.023	2571.8	2574.6	0.1725	0.5174
180	25	58.142	2661.5	2664.4	0.1235	0.5678
	20	62.977	2732.4	2735.3	0.0814	0.6141
	15	66.917	2787.9	2790.8	0.0471	0.6564
	10	70.205	2831.3	2834.2	0.0216	0.6950
	5	73.007	2865.2	2868.1	0.0056	0.7304
	0	75.440	2891.7	2894.6	6×10^{-12}	0.7632
	5	77.590	2912.6	2915.4	0.0061	0.7937
	10	79.521	2928.9	2931.8	0.0256	0.8223
	15	81.281	2941.7	2944.6	0.0610	0.8496
	20	82.909	2951.6	2954.5	0.1160	0.8757
0	25	84.437	2959.2	2962.1	0.1959	0.9010
	30	85.889	2964.7	2967.6	0.3086	0.9258
	35	87.288	2968.5	2971.4	0.4660	0.9504
	40	88.652	2970.7	2973.6	0.6865	0.9750
	45[a]	89.997	2971.5	2974.3	0.9945	0.9996

[a]The value of ψ actually used was 44.99°.

ples of the thickness period $D_0 = 2167$ Å and $D_{90} = 2976$ Å to the lower and upper limits, respectively, of each thickness branch, and considering the effect of overlapping, the band-structure diagram of Fig. 6 is generated. Figure 6 schematically gives the PTB (which are separated by forbidden gaps) where PSA-NE can be carried out on the SiO$_2$-Si system at $\lambda = 6328$ Å. Note that PSA-NE can be used for the SiO$_2$-Si system at 6328 Å for all oxide-film thicknesses greater than the lower edge (d_{3l}) of the third (and last) continuum PTB, i.e.,
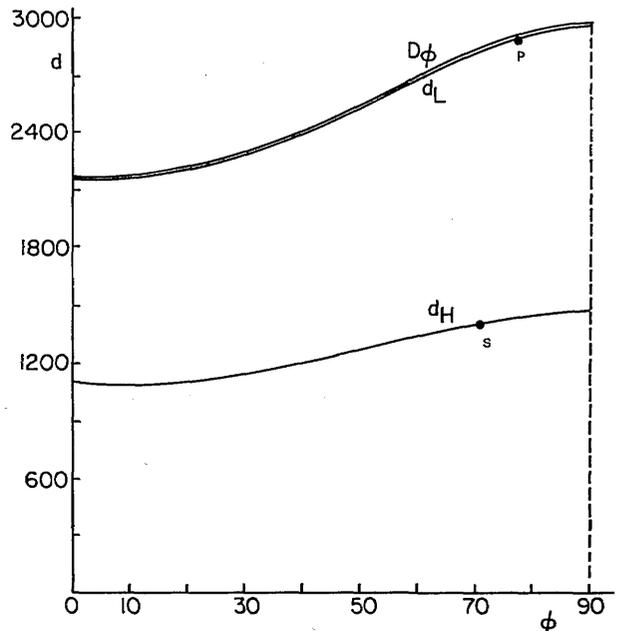

FIG. 5. The LPB and HPB, d_L and d_H, respectively, for the SiO$_2$-Si system at $\lambda = 6328$ Å. d_L and d_H are the loci of points (ϕ, d) in the reduced zone $(0 \leq d < D_\phi$, $0 \leq \phi \leq 90°)$ that lead to $\Delta = 0$ or π. $\psi = 0$ at P and 90° at S, corresponding to p- and s-suppression, respectively. Notice that $d_L \approx D_p$ and $d_H \approx \frac{1}{2} D_\phi$. This can be traced to the small extinction coefficient of Si at $\lambda = 6328$ Å. $d_L = D_\phi$, $d_H = \frac{1}{2} D_\phi$ hold exactly for an all-transparent ambient-film-substrate system.
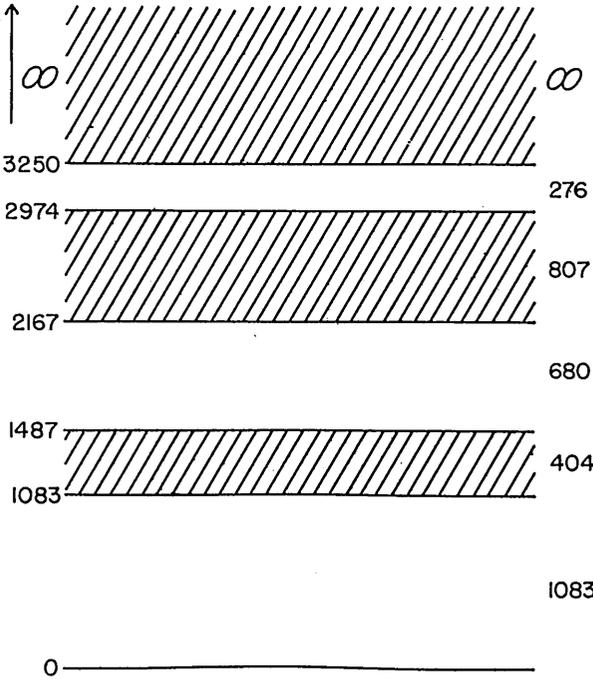
FIG. 6. Schematic of the structure of the PTB for PSA-NE on the SiO_2-Si system at $\lambda = 6328$ Å.

$d > 3250$ Å, which is about half the wavelength of light.

To summarize, the ranges of film thickness that permit PSA-NE on the SiO_2-Si system at $\lambda = 6328$ Å are

$$1083 < d < 1487 \text{ Å},$$
$$2167 < d < 2974 \text{ Å}, \tag{15}$$
$$d > 3250 \text{ Å}.$$

In the Appendix, we provide data for the SiO_2-Si system at selected mercury spectral lines to demonstrate the fact that PSA-NE can be used to determine virtually any film thickness by changing the wavelength of operation to avoid the forbidden gaps.

III. MULTIPLE PSA-NE MEASUREMENTS ON A FILM-SUBSTRATE SYSTEM OF A GIVEN FILM THICKNESS

We have determined in Sec. II the PTB for PSA-NE on a film–substrate system. The number of PSA-NE measurements and the angles of incidence at which they are realizable depend on the film thickness. In this section, we consider this aspect of the problem.

For a given film thickness d, the trajectory of the ellipsometric function $\rho(\phi, d)$ in the complex ρ plane as ϕ is varied from 0 to 90°, the so-called constant-thickness contour[4] (CTC), is unique to that thickness alone. In other words, no two CTC's $\rho(\phi, d_1)$ and $\rho(\phi, d_2)$ for film thickness d_1 and d_2, respectively, are ever identical unless $d_1 = d_2$, where $0 \le d < \infty$. Consequently, each and every thickness d leads to a different Δ-vs-ϕ curve with different set of intersection points (if any) with the $\Delta = \pi$ or 2π (0) lines.

For a given film–substrate system with known film thickness, the angles of incidence for PSA-NE can be
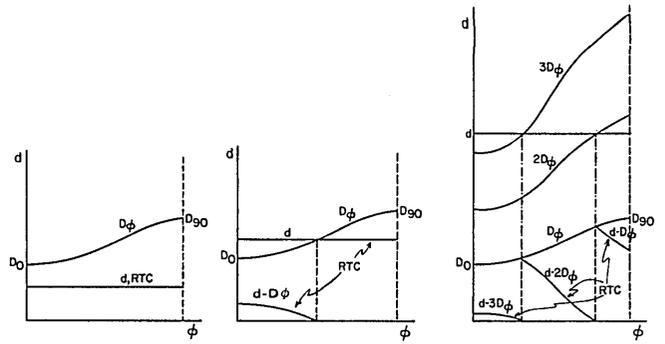

FIG. 7. The RTC for three choices of the film thickness. Left, $0 < d < D_0$; middle, $D_0 < d < D_{90}$; right: $d > mD_{90}$, where m is an integer.

conveniently and readily determined from the intersections of the HPB and LPB (Sec. II) with the reduced-thickness curve (RTC). The RTC is obtained by translating each point on the d = const (horizontal) line in the ϕd plane vertically downwards by a distance equal to the appropriate multiple of the thickness period D_ϕ at that point to bring it within the RTZ, below the D_ϕ curve. As shown in Fig. 7, the RTC depends on the film thickness d. If $d < D_0$, both the d = const line and the RTC are identical, Fig. 7-left. If $D_0 < d < D_{90}$, the RTC consists of two segments, a curved segment, $d - D_\phi$, and a horizontal straight-line segment that is coincident with the d = const line, Fig. 7-middle. In general, the RTC consists of several segments $d - mD_\phi$, $d - (m-1)D_\phi$, ... and resembles a saw-tooth curve, Fig. 7-right, with vertical transitions from one segment to the next when

$$d - kD_\phi = 0, \quad k = m, \quad m-1, \quad m-2, \ldots . \tag{16}$$

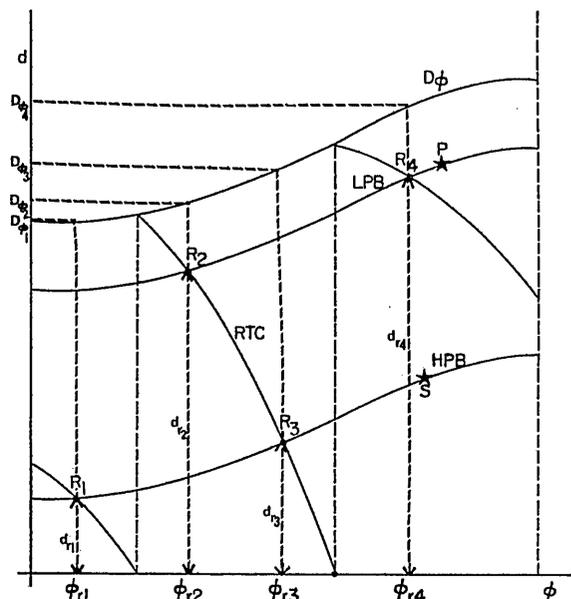In Fig. 8, the intersection points between the HPB and

FIG. 8. Construction for the determination of the angles of incidence at which PSA-NE is possible on a film–substrate system with a known film thickness.

LPB; and the RTC R_1, R_2, ... define the angles of incidence ϕ_{r1}, ϕ_{r2}, ... for PSA-NE. Note that the ellipsometric angle ψ alternates between the high ($\psi > 45°$) and the low ($\psi < 45°$) values at the successive intersections. Thus, if all odd-numbered intersections have $\psi > 45°$, then all even-numbered intersections will have $\psi < 45°$, and vice versa. The ellipsometric angle Δ is either π or 0, dependent on whether the intersection point R lies to the left or to the right of the point S (where $\psi = 90°$) on the HPB, or the point P (where $\psi = 0$) on the LPB. (In Fig. 8, $\Delta = \pi$ at all intersections.)

IV. MEASUREMENT OF FILM THICKNESS OF A TRANSPARENT FILM ON A SUBSTRATE BY PSA-NE

One important and straightforward application of PSA-NE is to determine the film thickness of a transparent film on an absorbing substrate when the refractive indices of the film and the substrate are known. An example is the determination of the thickness of silicon dioxide and other transparent films involved in the integrated-circuit technology. It is significant to observe that the range of film thickness that permits such well-known interferometric reflectance methods as the CARIS (constant-angle reflection interference spectroscopy) and VAMFO (variable-angle monochromatic fringe observation)[11] would also allow PSA-NE. The oscillatory behavior of the Δ-vs-ϕ curve, observed when the film thickness exceeds a certain minimum value (about half the wavelength), arises from the same interference effect that leads to oscillatory reflectance curves.

From the given refractive indices of the film and substrate, and the wavelength of measurements, the HPB and LPB are computed (Sec. II). This need be done only once; the results are used whenever any unknown thickness needs to be measured. The quantities that need to be measured in PSA-NE are the angles of incidence ϕ_{r1}, ϕ_{r2}, ... at the nulls, and a determination of whether ψ is greater or less than $45°$ at each null. This accounts for considerable simplification in the operation of the instrument (see Sec. V). From ϕ_{r1}, ϕ_{r2}, ... and whether ψ is high ($\psi > 45°$) or low ($\psi < 45°$), the points of intersection R_1, R_2, ... of the RTC for the unknown thickness d with the HPB and LPB are determined (see Fig. 8). Let $(d_{r1}, D_{\phi r1})$, $(d_{r2}, D_{\phi r2})$, ... indicate the reduced film thickness (the ordinate of the HPB or LPB) and film-thickness period, respectively, evaluated at the successive nulling angles of incidence ϕ_{r1}, ϕ_{r2}, ... Then from the definition of the reduced thickness, we have

$$d = d_{ri} + kD_{\phi ri},$$
$$i = 1, 2, 3, \ldots,$$
$$k = \begin{cases} M, & M-1, & M-1, & M-2, & M-2, & \ldots \\ M, & M, & M-1, & M-1, & M-2, & M-2, & \ldots \end{cases}$$
(17)

In Eqs. (17), k is an integer that is the same for each segment of the saw-tooth RTC, and decreases by 1 at each transition between one segment and the next. The maximum value of k is M, which applies to the first segment of the RTC, see Fig. 8.

From Eqs. (17), it is clear that only two null mea-

surements at two successive angles of incidence need to be made. Two cases can be distinguished, (a) if the first of the two successive measurements gives a low-psi value ($0 < \psi < 45°$), the two measurements will have to correspond to intersections of the same segment of the RTC with LPB and HPB; (b) on the other hand, if the first measurement gives a high-psi value ($45° < \psi < 90°$), the two measurements will correspond to intersections of two successive segments of the RTC with the HPB and LPB, respectively. With k the same for both measurements in case (a), solving two of Eqs. (17) gives

$$d = \left(\frac{d_1}{D_1} - \frac{d_2}{D_2}\right) \bigg/ \left(\frac{1}{D_1} - \frac{1}{D_2}\right).$$
(18a)

With k different by 1 for the two measurements in case (b), solving two of Eqs. (17) gives

$$d = d_1 + \frac{D_1[D_2 - (d_2 - d_1)]}{(D_2 - D_1)}.$$
(18b)

Equations (18) provide the required film thickness from measurements of two successive angles of incidence ϕ_1, ϕ_2 ($\phi_2 > \phi_1$) in terms of the reduced thicknesses d_1, d_2 and the film-thickness periods D_1, D_2 evaluated at these angles.

A simpler situation exists when we know an approximate range for the unknown film thickness. In this case, only one PSA null measurement needs to be made. The reduced thickness d_r at the nulling angle of incidence is simply increased by the multiple of the film-thickness period D_ϕ (evaluated at that angle) that brings the thickness within the given range. This yields the film thickness required. By requiring only one PSA null measurement, the range of applicability of this method of thickness measurements includes the entirety of the PTB.

When the film is thick enough to make possible multiple PSA null measurements at several angles of incidence, an accurate value for the film thickness can be obtained by a least-square solution for d (and k) of the overdetermined set of Eqs. (17).

V. PSA NULL ELLIPSOMETER

The arrangement of the optical components of the PSA ellipsometer is rather simple (Fig. 1). The method of obtaining the null is to set either the polarizer P or the analyzer A at a fixed azimuth from the plane of incidence (other than 0 or $\pi/2$) and to adjust the azimuth of the other element, together with the angle of incidence ϕ until the light transmitted by the PSA sequence of elements is extinguished. For ease of operation, the sample table should be geared to rotate at half the rate of rotation of the analyzer telescope, to keep the reflected beam along the analyzer-telescope axis. If P and A are the nulling polarizer and analyzer azimuths,

$$\tan\psi = \mp \tan P \tan A,$$
(19)

where the $-$ and $+$ signs correspond to $\Delta = 0$ and $\Delta = \pi$, respectively. If the polarizer azimuth is $P = 45°$, Eq. (19) becomes

$$\tan\psi = \mp \tan A,$$

so that

$$\psi = \pi - A, \quad \text{when } \Delta = 0$$

$$\psi = A, \qquad \text{when } \Delta = \pi. \tag{20}$$

From Eqs. (20), we find that A lies in the ranges

$$0 < A < 45°, \qquad 135° < A < 180°, \quad \text{when } 0 < \psi < 45°,$$

$$45° < A < 135°, \quad \text{when } 45° < \psi < 90°. \tag{21}$$

Figure 9 shows a schematic of these low-psi and high-psi quadrants for the analyzer transmission axis. We have seen in Sec. IV that, when the film thickness is to be determined, we need only to know whether $\psi < 45°$ or $\psi > 45°$, i.e., the quadrant in which the analyzer is located at null, without requiring the actual value of ψ. Therefore, the only data are the angle of incidence ϕ and this quadrant information on the analyzer position at null.

The operation of the PSA-NE can be readily automated by providing motor drives for the angle-of-incidence goniometer and for the analyzer (or polarizer). For film-thickness measurements (Sec. IV), we need only quadrant readout for the analyzer position, so that the angles of incidence at the successive nulls represent the primary information in this case. The procedure would be to scan the angle of incidence ϕ over as large a segment of the total range $0 \le \phi \le 90°$ as possible, and to hunt for all of the nulls in that range.

The PSA ellipsometer can also be operated in the rotating-analyzer mode.[12-16] In this case, the analyzer is rotated synchronously and the angle of incidence is scanned to determine the angles at which the reflected light is linearly polarized, as evidenced by maximum (unity) modulation of the detector current. Automation in this mode is much simpler than in the nulling mode, because the rotating-analyzer mode involves a single direct scan of the angle of incidence, whereas an interactive succession of alternating small steps of both the angle of incidence and analyzer azimuth are needed for null convergence.
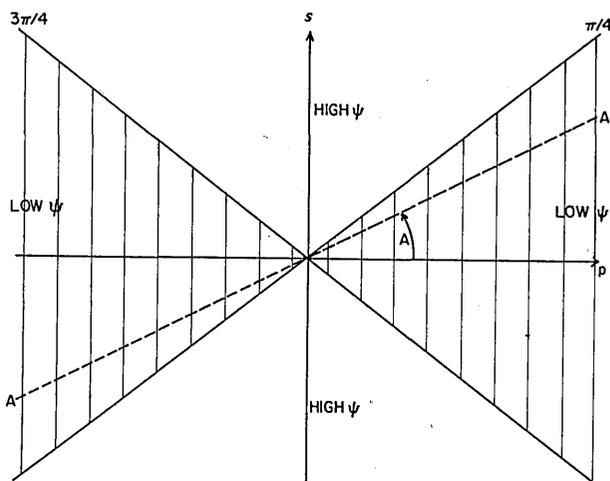

FIG. 9. The high- and low-psi quadrants of the analyzer transmission axis when the polarizer is set at an azimuth $P = 45°$.

TABLE III. The PTB for PSA-NE on the SiO_2-Si film–substrate system at selected mercury spectral lines.

Wavelength λ (Å)	First permissible base–band limits (Å)	Second permissible base–band limits (Å)	Lower limit of the continuum band (higher limit is ∞) (Å)
5461	941–1298	1880–2597	2825
4358	745–1020	1487–2041	2238
4046	687–932	1365–1866	2064
3650	611–808	1180–1625	1849
3341	551–715	1042–1444	1680
3131	514–659	962–1332	1567
2537	410–475	677–973	1256

VI. EXPERIMENTAL

PSA-NE was used to determine the film thickness of silicon dioxide films on silicon wafer of the type used in integrated-circuit technology. An ordinary ellipsometer was employed, by simply removing the compensator. The procedure was to set the polarizer at a fixed azimuth and to adjust the angle of incidence ϕ and analyzer azimuth A for null. The nulls thus obtained were very well defined.[17]

On one sample, with $P = 140.55°$, two nulls were obtained at angles of incidence $\phi_{r1} = 26.122°$ and $\phi_{r2} = 48.353°$ at $\lambda = 6328$ Å. The corresponding analyzer null azimuths were $132.648°$ and $118.696°$, indicating low ($< 45°$) and high ($> 45°$) values of ψ at these two angles, respectively. At ϕ_{r1}, ϕ_{r2}, the computed reduced film thicknesses d_{r1}, d_{r2} and the film-thickness periods $D_{\phi r1}$, $D_{\phi r2}$ [see Secs. III and IV] were (2263, 1265 Å) and (2266, 2534 Å), respectively. Substitution of these values into Eq. (18a) yielded a film thickness $d = 10 \, 701$ Å, which checked well with the nominal thickness given by the manufacturer (10 000 Å) for the wafer. The difference between the measured and nominal film thicknesses can be attributed, at least in part, to a possible error of the assumed optical constants for the SiO_2-Si system.

APPENDIX

In measuring the film thickness of a film–substrate system by PSA-NE, the forbidden gaps may be a problem. We can overcome this by changing the wavelength. In general, we shift the forbidden-gap position on the film-thickness scale by changing the wavelength.

Table III gives the PTB for the SiO_2-Si film–substrate system at selected mercury spectral lines. From this table, a film thickness of $d = 1500$ Å lies in a forbidden gap at $\lambda = 5461$ Å. If λ is changed to 4358 Å, the thickness becomes within the second permissible base band, so that PSA-NE becomes possible.

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[2]H. M. O'Bryan, J. Opt. Soc. Am. 26, 122 (1936). In this paper, O'Bryan mentions the similarity of his idea to that of Brewster, who over a century earlier [Philos. Trans. 69, 133 (1830)] observed that light multiply reflected between a pair of parallel mirrors can be extinguished between two Nicol prisms. In this case, the phase shift per reflection is π/M, so that for M reflections, the cummulative shift is $(\pi/M) \times M = \pi$.

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[6]See Eq. (13) and Fig. 3 of Ref. 4.

[7]s or p suppression refers to the total extinction of the s or p components of the incident light upon reflection and identifies the condition when the film—substrate system acts as a reflection polarizer.

[8]The vertical translation of a base band by a multiple of the thickness period preserves the range of ψ (high or low).

[9]Note the difference of notation between d_l^{1m} and d_{ml}
d_l^{1m} indicates the lower edge of a translated band, whereas d_{ml} is the lower edge of a higher band. A translated band

may or may not constitute a higher band, dependent on the overlapping of all translated bands.

[10]*Ellipsometric Tables of the* Si–SiO$_2$ *System for Mercury and* He–Ne *Laser Spectral Lines*, edited by G. Gergely (Akademiai Kiado, Budapest, 1971).

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[17]An important parameter for the precise determination of the null by the PSA ellipsometer is the value of the derivative $\partial\Delta/\partial\phi$ at the nulling angle ϕ. This derivative determines how rapidly the reflected light becomes elliptically polarized as the angle of incidence is offset from its null position. An initial investigation shows a tendency for high values of $\partial\Delta/\partial\phi$ at null, in most cases, leading to very precise null definition.