12-1975

Polarizer-surface-analyzer null ellipsometry for film-substrate systems

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

A.-R. M. Zaghloul

N. M. Bashara

Follow this and additional works at: https://scholarworks.uno.edu/ee_facpubs

Part of the Electrical and Electronics Commons, and the Physics Commons

Recommended Citation
Polarizer–surface-analyzer null ellipsometry for film–substrate systems

R. M. A. Azzam, A.-R. M. Zaghloul, and N. M. Bashara

Electrical Materials Laboratory, College of Engineering, University of Nebraska, Lincoln, Nebraska 68508
(Received 13 June 1975)

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 \( \rho \) (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 SiO2-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 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, \( \delta_p \) and \( \delta_s \), respectively. The difference between these phase shifts, \( \Delta = \delta_p - \delta_s \), is generally neither \( 0 \) nor \( \pi \) for angles of incidence \( 0 < \phi < 90^\circ \), 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 \( \Delta \). This is the basis of two commonly used (PCSA and PSCA) null-ellipsometer arrangements.

It is obvious that if \( \Delta = 0 \) or \( \pi \) at oblique incidence, no compensator would be needed and PSA null ellipsometry (PSA-NE) can be used. The condition \( \Delta = 0 \) or \( \pi \) 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 \( \pi \), O'Bryan developed an ingenious method. O'Bryan exploited the fact that \( \Delta \) 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.

In this paper, we show that single-pass PSA-NE can be used to characterize film-substrate systems, provided that the film thickness lies within certain permissible-thickness bands (PTB). This possibility has been recently discovered; here we elaborate on it. For the purpose of illustration, we take the SiO2-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 \( \Delta \) AS A FUNCTION OF THE ANGLE OF INCIDENCE \( \phi \) FOR A FILM-SUBSTRATE SYSTEM

For a bare substrate (Si) the reflection phase difference \( \Delta \) is a monotonically decreasing function of the angle of incidence \( \phi \), falling from \( \pi \) at \( \phi = 0 \) (normal incidence) to \( 0 \) at \( \phi = 90^\circ \) (grazing incidence), Fig. 2-left (continuous curve). The presence of a very-thin film (SiO2; \( d = 20 \) Å) does not change the monotonic character of the \( \Delta \)-vs-\( \phi \) curve, Fig. 2-left (dashed curve). However, as the thickness \( d \) of the transparent film (SiO2) is increased beyond a certain minimum value, the monotonic nature of the \( \Delta \)-vs-\( \phi \) curve ceases and gives way to an oscillatory (non-monotonic) behavior with one or more intersections of the curve with the \( \Delta = \pi \) or \( 2\pi \) (0)
In the following section, we arrive at the very interesting conclusion that the \( \Delta \)-vs-\( \phi \) curve is oscillatory and has intersections with the \( \Delta = \pi \) or \( 2 \pi \) (0) lines when the film thickness \( d \) lies within any one of a set of PTB:

\[
d_{L1} < d < d_{L2}, \quad i = 1, 2, 3, \ldots, L,
\]

where \( d_{L1} \) and \( d_{L2} \) represent the lower and upper limits of the \( i \)th band, respectively. Furthermore, we find that the upper thickness limit of the last (upper-most) thickness band, \( d_{Lm} \), is infinity (\( d_{Lm} = \infty \)) so that the top band is actually a continuum. A film-thickness value in the finite bands, \( d_{L1} < d < d_{L2}, \quad i = 1, 2, 3, \ldots, L - 1 \), and in the infinite continuum band, \( d > d_{L2} \),

leads to an oscillatory \( \Delta \)-vs-\( \phi \) curve with one or more intersections with the \( \Delta = \pi \) or \( \Delta = 0 \) \((2\pi)\) lines at oblique angles of incidence \( \phi \) \((\iota = 1, 2, \ldots)\), \( 0 < \phi < 90^\circ \). 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 \( \Delta \)-vs-\( \phi \) curve with zero initial slope at \( \phi = 0 \), \( \Delta \partial \phi = 0 \), is obtained. This situation is represented in Fig. 2-right \((d = d_{L2} = 2167 \, \text{Å})\).

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 \( \lambda = 6328 \, \text{Å} \).

Origin of the PTB

The quantity measured by an ellipsometer is the ratio

\[
\rho = R_p/R_s
\]

of the complex amplitude-reflection coefficients \( R_p \) and \( R_s \) of an optically isotropic surface for the parallel (\( \rho \)) and perpendicular (\( s \)) polarizations. In Ref. 4, we investigated the behavior of the ellipsometric function \( \rho \) for a film-substrate system as the angle of incidence \( \phi \) and the film thickness \( d \) are permitted to scan their entire ranges \( 0 \leq \phi \leq 90^\circ \), and \( 0 \leq d \leq \infty \), respectively. Figure 3 shows the complex plane of the ellipsometric function \( \rho \) (left), and the real plane of its two arguments \( \phi \) and \( d \) (right). At a fixed angle of incidence \( \phi \), if the thickness \( d \) of a transparent film is increased from zero, the point \( \rho \) moves, in the complex plane, from \( B \) on the zero-thickness contour \((ZTC)\) which represents the bare substrate, along a closed constant-angle-of-incidence contour \((CAIC)\). 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 \( \rho \) back to its initial position \( B \) when \( d = d_B \), which is the angle-of-incidence-dependent film-thickness period \((d\phi)\) of the function \( \rho(\phi, d) \). Because \( \rho \) is a real number at both \( H \) and \( L \), linearly polarized light of arbitrary azimuth, incident at a fixed angle of incidence \( \phi \) on a substrate covered by a transparent film, is reflected linearly polarized at two discrete film thicknesses \( d_H \) and \( d_L \), where

\[
0 < d_H < d_L < D_0.
\]

Because \( \rho \) is a periodic function of \( d \), with period \( D_0 \), we can generalize by saying that the reflected light becomes linearly polarized twice, at \( d = d_H + mD_0 \) and \( d = d_L + mD_0 \), as the film thickness \( d \) scans each period

\[
mD_0 < d < (m + 1)D_0, \quad m = 0, 1, 2, 3, \ldots
\]

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

FIG. 2. Left. Monotonic \( \Delta \)-vs-\( \phi \) curves for a bare substrate \((Si; \) continuous line) and a substrate \((Si\) covered by a very thin film \((SiO_2; 20 \, \text{Å}; \) dashed line) \((\lambda = 6328 \, \text{Å})\). Middle. Oscillatory \( \Delta \)-vs-\( \phi \) curve for a film-substrate \((SiO_2-Si)\) system with film thickness \((d = 1200 \, \text{Å})\) in a PTB \((\lambda = 6328 \, \text{Å})\). Right. Monotonic \( \Delta \)-vs-\( \phi \) curve for a film-substrate \((SiO_2-Si)\) system with a film thickness \((d = 2167 \, \text{Å})\) that corresponds to a band edge \((\lambda = 6328 \, \text{Å})\).

FIG. 3. Mapping between the complex plane of the ellipsometric function \( \rho \) (left) and the plane of its two real arguments; the angle of incidence \( \phi \) 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 \( \rho \) plane is mapped into a closed contour in the \( \rho d \) plane, NSGPN. The origin of the PTB for PSA-NE is explained with the help of this figure.
whose lower and upper limits are given by Eqs. (12) are overlapping and merge into one base band general notation of Sec. I, we have 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 angles of incidence, i.e.,

\[ |p_H| > 1, \quad 45° < \psi_H \leq 90°, \]

and for L,

\[ |p_L| < 1, \quad 0 \leq \psi_L < 45°, \]

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

\[ 0 \leq d < d_{90}, \quad 0 \leq \phi \leq 90°, \]

of the \( \phi d \) plane correspond to high-\( \psi \) (45° < \( \psi \) < 90°) and low-\( \psi \) (0 < \( \psi < 45° \)) 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, \( NP, \Delta = 0 \); and on the other, \( PG, \Delta = 0 \). The entire real axis of the \( \rho \) plane, \( NSGPN \) (Fig. 3-left), is mapped into a closed contour in the \( \phi d \) 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 \( \phi d \) plane are mapped onto the single points \( N (\rho = -1) \) and \( G (\rho = 1) \), respectively, in the \( \rho \) plane.]

Let \( d_{90} \) and \( d_{90H} \) be the lower and upper thickness limits of the HPB, \( d_H \), at \( \phi = 0 \) and 90°, respectively; and let \( d_{90L} \) and \( d_{90L} \) be the corresponding thickness limits for the LPB, \( d_L \). Although the thickness gap,

\[ \Delta d_o = d_L - d_H, \]

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

\[ \Delta d_o > 0, \quad 0 \leq \phi \leq 90°, \]

two cases, Fig. 4, can be distinguished:

case 1, \( d_{90L} \geq d_{90H} \),

\[ (11a) \]

case 2, \( d_{90L} \leq d_{90H} \).

\[ (11b) \]

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

\[ d_{90L} \leq d_H \leq d_{90H}, \quad d_{90L} \leq d_L \leq d_{90L}, \]

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

\[ d_{11} = d_{90L}, \quad d_{1u} = d_{90H}; \]

\[ (13a) \]

\[ d_{21} = d_{90L}, \quad d_{2u} = d_{90H}. \]

\[ (13b) \]

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

\[ d_{11} = d_{90}, \quad d_{1u} = d_{90L}. \]

\[ (13b) \]

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 \( \rho \) 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. Thus the thickness limits of a band obtained from translating base band 1 by adding \( n \) thickness periods are

\[ d_{1m} = d_{11} + mD_0, \quad d_{1u} = d_{1u} + mD_{90}. \]

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

\[ d_{2m} = d_{21} + nD_0, \quad d_{2u} = d_{2u} + nD_{90}. \]

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 \( m_{\text{max}} \) and \( n_{\text{max}} \), 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 \( \rho \) 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 \( \rho \) 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

\[ \text{FIG. 4. The cases of (1) separate (left), and (2) overlapping (right) permissible base bands. In case (2) (right), the two base bands merge together to form one permissible band.} \]
angle of incidence $\phi$ and the film thickness $d$ that realize any given value of $\rho$ 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.

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

The value of $\phi$ actually used was 44.99°.

Values of $\rho$ that correspond to points in the different regions of the real axis marked in Fig. 3-left were calculated from Eq. (6), with $\phi$ taken between 0 and 90° in steps of 5° and $\Delta = 0$ or $\pi$. These values were subsequently substituted into Eq. (25) of Ref. 3 and the corresponding angle of incidence $\phi$ 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 $\Delta$ and $\phi$, and columns 3 and 4 give the angle of incidence $\phi$ and the least film thickness $d$ (equal to $d_{4\phi}$ or $d_L$). For completeness, we list the thickness period $D_{0\phi}$ and the $p$ and $s$ reflectances $\rho_p$ and $\rho_s$ in columns 5, 6, and 7, respectively, of Tables I and II.

Figure 5 shows a plot of the two branches $(\phi, d_{4\phi})$ and $(\phi, d_L)$ in the $\phi d$ plane. The lower and upper thickness limits of the HPB and LPB are $d_{4\phi} = 1083$ Å and $d_{4\phi} = 1487$ Å; and $d_{Lp} = 2164$ Å and $d_{Ls} = 2973$ Å. Note that $d_{4\phi} > d_{4\phi}$ [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 $\phi$ and reduced film thickness $d$ for a SiO$_2$-Si film-substrate system at $\lambda = 6328$ Å that lead to $\Delta = 0$ or $\pi$ (thus allowing PSA-NE) for different values of $\phi$ in the range $45^\circ < \phi < 90^\circ$ (HPB). $D_{4\phi}$ is the film-thickness period and $\rho_p$ and $\rho_s$ are the $p$ and $s$ reflectances.

<table>
<thead>
<tr>
<th>$\Delta$ (deg.)</th>
<th>$\phi$ (deg.)</th>
<th>$d_L$ (Å)</th>
<th>$D_{4\phi}$ (Å)</th>
<th>$\rho_p$</th>
<th>$\rho_s$</th>
</tr>
</thead>
<tbody>
<tr>
<td>45°</td>
<td>2.362</td>
<td>1083.2</td>
<td>2168.0</td>
<td>0.0826</td>
<td>0.6235</td>
</tr>
<tr>
<td>50</td>
<td>37.860</td>
<td>1193.2</td>
<td>2388.4</td>
<td>0.0975</td>
<td>0.6868</td>
</tr>
<tr>
<td>55</td>
<td>46.764</td>
<td>1249.2</td>
<td>2500.7</td>
<td>0.1136</td>
<td>0.6557</td>
</tr>
<tr>
<td>60</td>
<td>52.414</td>
<td>1386.1</td>
<td>2693.7</td>
<td>0.1310</td>
<td>0.6537</td>
</tr>
<tr>
<td>65</td>
<td>56.760</td>
<td>1355.0</td>
<td>2642.5</td>
<td>0.1500</td>
<td>0.6236</td>
</tr>
<tr>
<td>70</td>
<td>62.977</td>
<td>1397.2</td>
<td>2773.7</td>
<td>0.1939</td>
<td>0.6213</td>
</tr>
<tr>
<td>75</td>
<td>66.917</td>
<td>1386.1</td>
<td>2773.7</td>
<td>0.2197</td>
<td>0.6236</td>
</tr>
<tr>
<td>80</td>
<td>70.265</td>
<td>1430.2</td>
<td>2808.8</td>
<td>0.2487</td>
<td>0.6213</td>
</tr>
<tr>
<td>85</td>
<td>73.197</td>
<td>1417.7</td>
<td>2828.6</td>
<td>0.2817</td>
<td>4 $\times 10^{-12}$</td>
</tr>
<tr>
<td>90</td>
<td>75.560</td>
<td>1410.7</td>
<td>2828.6</td>
<td>0.3197</td>
<td>0.6236</td>
</tr>
</tbody>
</table>

**Table II.** Same as in Table I but for $\phi$ in the range $0 \leq \phi < 45^\circ$ (LPB).

<table>
<thead>
<tr>
<th>$\Delta$ (deg.)</th>
<th>$\phi$ (deg.)</th>
<th>$d_L$ (Å)</th>
<th>$D_{4\phi}$ (Å)</th>
<th>$\rho_p$</th>
<th>$\rho_s$</th>
</tr>
</thead>
<tbody>
<tr>
<td>45°</td>
<td>1.487</td>
<td>2164.7</td>
<td>2167.5</td>
<td>0.3452</td>
<td>0.3454</td>
</tr>
<tr>
<td>40</td>
<td>32.112</td>
<td>2324.8</td>
<td>2328.6</td>
<td>0.8285</td>
<td>0.4051</td>
</tr>
<tr>
<td>35</td>
<td>43.914</td>
<td>2495.9</td>
<td>2492.8</td>
<td>0.2270</td>
<td>0.4629</td>
</tr>
<tr>
<td>30</td>
<td>52.023</td>
<td>2571.8</td>
<td>2574.6</td>
<td>0.1725</td>
<td>0.5147</td>
</tr>
<tr>
<td>25</td>
<td>60.142</td>
<td>2661.5</td>
<td>2664.4</td>
<td>0.1235</td>
<td>0.5678</td>
</tr>
<tr>
<td>20</td>
<td>69.977</td>
<td>2732.4</td>
<td>2735.3</td>
<td>0.0614</td>
<td>0.6141</td>
</tr>
<tr>
<td>15</td>
<td>76.917</td>
<td>2787.9</td>
<td>2789.0</td>
<td>0.0471</td>
<td>0.6664</td>
</tr>
<tr>
<td>10</td>
<td>80.265</td>
<td>2831.3</td>
<td>2834.2</td>
<td>0.0216</td>
<td>0.6950</td>
</tr>
<tr>
<td>5</td>
<td>73.007</td>
<td>2865.2</td>
<td>2866.1</td>
<td>0.0066</td>
<td>0.7504</td>
</tr>
<tr>
<td>0</td>
<td>75.460</td>
<td>2891.7</td>
<td>2894.6</td>
<td>6 $\times 10^{-12}$</td>
<td>0.7632</td>
</tr>
</tbody>
</table>

*The value of $\phi$ actually used was 45°.1°.

**Figure 5.** The LPB and HPB, $d_L$ and $d_{4\phi}$, respectively, for the SiO$_2$-Si system at $\lambda = 6328$ Å. $d_L$ and $d_{4\phi}$ are the loci of points $(\phi, d)$ in the reduced zone ($0 < d < D_{4\phi}$) that lead to $\Delta = 0$ or $\pi$, $\phi = 0$ at $P$ and $90^\circ$ at $S$, corresponding to $p$- and $s$-polarization, respectively. Notice that $d_{4\phi} = D_{4\phi}$ and $d_L = \frac{1}{2} D_{4\phi}$ 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

$$1083 < d < 1487$$ Å,

$$2167 < d < 2974$$ Å,

$$d > 3250$$ Å.  

(15)

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 $\rho$ plane as $\phi$ is varied from 0 to 90°, the so-called constant-thickness contour (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 $0 \leq d < \infty$. Consequently, each and every thickness $d$ leads to a different $\Delta$-vs-$\phi$ curve with different set of intersection points (if any) with the $\Delta = \pi$ or $2\pi$ (0) lines.

For a given film-substrate system with known film thickness, the angles of incidence for PSA-NE can be 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 $\phi d$ plane vertically downwards by a distance equal to the appropriate multiple of the thickness period $D_0$ at that point to bring it within the RTZ, below the $D_0$ 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, $d - D_0$, 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 $d - mD_0$, $d - (m - 1)D_0$, ... and resembles a saw-tooth curve, Fig. 7-right, with vertical transitions from one segment to the next when

$$d - kD_0 = 0, \quad k = m, \quad m - 1, \quad m - 2, \ldots.$$

(16)

In Fig. 8, the intersection points between the HPB and...
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) 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 φ₁, φ₂, ..., 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 φ₁, φ₂, ..., and whether ψ is high (ψ > 45°) or low (ψ < 45°), the points of intersection R₁, R₂, ..., of the RTC for the unknown thickness d with the HPB and LPB are determined (see Fig. 8). Let (d₁₁, D₀₁), (d₂₂, D₀₂), ... 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 φ₁, φ₂, .... Then from the definition of the reduced thickness, we have

\[ d = d_{ri} + kD_{or1}, \]

\[ i = 1, 2, 3, \ldots \]

\[ k \in \{M, M-1, M-2, M-3, \ldots \} \]

(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 measurements 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 < ψ < 45°), the two measurements will have to correspond to intersections of the same segment of the RTC with HPB and LPB; (b) on the other hand, if the first measurement gives a high-psi value (45° < ψ < 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

\[ d = \frac{(d_1 - d_2)}{(1 - \frac{1}{D_1})}. \]

(18a)

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

\[ d = d_{r1} + \frac{D_2 - (d_2 - d_1)}{(D_2 - D_1)}. \]

(18b)

Equations (18) provide the required film thickness from measurements of two successive angles of incidence φ₁, φ₂ in terms of the reduced thicknesses d₁, d₂ and the film-thickness periods D₁, D₂ 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 d₁ at the nulling angle of incidence is simply increased by the multiple of the film-thickness period D₀ (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 π/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 Δ = 0 and Δ = π, respectively. If the polarizer azimuth is P = 45°, Eq. (19) becomes

\[ \tan \psi = \mp \tan A, \]
so that

\[ \psi = \pi - \Delta, \quad \text{when } \Delta = 0 \]

\[ \psi = \Delta, \quad \text{when } \Delta = \pi. \]

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

\[ 0 < \theta < 45^\circ, \quad 135^\circ < \theta < 180^\circ, \quad \text{when } 0 < \psi < 45^\circ, \]

\[ 45^\circ < \theta < 135^\circ, \quad \text{when } 45^\circ < \psi < 90^\circ. \]

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 \( \psi < 45^\circ \) or \( \psi > 45^\circ \), i.e., the quadrant in which the analyzer is located at null, without requiring the actual value of \( \psi \). Therefore, the only data are the angle of incidence \( \phi \) 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 \( \phi \) over as large a segment of the total range \( 0 \leq \phi \leq 90^\circ \) 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.

![Figure 9](image)

**FIG. 9.** The high- and low-psi quadrants of the analyzer transmission axis when the polarizer is set at an azimuth \( P = 45^\circ \).

### Table III. The PTB for PSA-NE on the SiO₂-Si film-substrate system at selected mercury spectral lines.

<table>
<thead>
<tr>
<th>Wavelength (Å)</th>
<th>First permissible base-band limits (Å)</th>
<th>Second permissible base-band limits (Å)</th>
<th>Lower limit of the continuum band (higher limit is ( \infty )) (Å)</th>
</tr>
</thead>
<tbody>
<tr>
<td>5461</td>
<td>941–1239</td>
<td>1860–2597</td>
<td>2525</td>
</tr>
<tr>
<td>4358</td>
<td>745–1020</td>
<td>1497–2041</td>
<td>2338</td>
</tr>
<tr>
<td>4046</td>
<td>687–932</td>
<td>1360–1666</td>
<td>2064</td>
</tr>
<tr>
<td>3650</td>
<td>611–806</td>
<td>1160–1625</td>
<td>1849</td>
</tr>
<tr>
<td>3361</td>
<td>551–715</td>
<td>1043–1444</td>
<td>1680</td>
</tr>
<tr>
<td>3131</td>
<td>514–659</td>
<td>965–1332</td>
<td>1567</td>
</tr>
<tr>
<td>2537</td>
<td>410–475</td>
<td>677–973</td>
<td>1356</td>
</tr>
</tbody>
</table>

### 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 \( \phi \) and analyzer azimuth \( A \) for null. The nulls thus obtained were very well defined.17

On one sample, with \( P = 140.55^\circ \), two nulls were obtained at angles of incidence \( \phi_1 = 26.122^\circ \) and \( \phi_2 = 48.353^\circ \) at \( \lambda = 6328 \) Å. The corresponding analyzer null azimuths were 132.848° and 118.986°, indicating low (\( < 45^\circ \)) and high (\( > 45^\circ \)) values of \( \psi \) at these two angles, respectively. At \( \phi_1, \phi_2 \), 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 \( d = 10701 \) 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 SiO₂-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 SiO₂-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 \( \lambda \) is changed to 4358 Å, the thickness becomes within the second permissible base band, so that PSA-NE becomes possible.

*Supported by the National Science Foundation.

† Also with the Division of Hematology, Department of Internal Medicine, College of Medicine, University of Nebraska Medical Center, Omaha, Neb. 68105.

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 $\pi/M$, so that for $M$ reflections, the cumulative shift is $(\pi/M) \times M = \pi$.


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

$s$ 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.

The vertical translation of a base band by a multiple of the thickness period preserves the range of $\psi$ (high or low).

Note the difference of notation between $d^i_m$ and $d^i_{si}$. $d^i_m$ indicates the lower edge of a translated band, whereas $d^i_{si}$ 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.


An important parameter for the precise determination of the null by the PSA ellipsometer is the value of the derivative $\partial A/\partial \phi$ at the nulling angle $\phi$. 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 $\partial A/\partial \phi$ at null, in most cases, leading to very precise null definition.