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Constant-psi constant-delta contour maps: applications to ellipsometry and to reflection-type optical devices

A.-R. M. Zaghloul and R. M. A. Azzam

Constant-psi constant-delta contour maps in the reduced angle-of-incidence–film-thickness plane that are useful in ellipsometry and in design of reflection-type optical devices are discussed. As a specific example, a contour map is given for the SiO$_2$–Si film–substrate system at the 6328-Å He–Ne laser wavelength.

I. Introduction

When light is obliquely reflected from a homogeneous semi-infinite parallel–plane film–substrate system, the two components of its electric vector vibrating parallel ($p$) and perpendicular ($s$) to the plane of incidence undergo different amplitude and phase changes. With reference to Fig. 1, $N_0$, $N_1$, and $N_2$ are the (complex) refractive indices of the ambient (0), film (1), and substrate (2), respectively. $d$ and $\phi$ are the film thickness and angle of incidence, respectively. The complex reflection coefficients $R_p$ and $R_s$, that relate the amplitudes and phases of the incident and reflected beams for each polarization component, are given by

$$ R_p = \frac{r_{01p} + r_{12p} \exp(-j2\beta)}{1 + r_{01p}r_{12p} \exp(-j2\beta)}, $$

$$ R_s = \frac{r_{01s} + r_{12s} \exp(-j2\beta)}{1 + r_{01s}r_{12s} \exp(-j2\beta)}, $$

$$ \beta = 2\pi(d/\lambda)(N_1^2 - N_2^2 \sin^2\phi)^{1/2}, $$

where $r_{01p}$ ($r_{01s}$) and $r_{12p}$ ($r_{12s}$) are the 01 and 12 interface reflection coefficients for the $p$ ($s$) components. The ellipsometric function $\rho$ of the film–substrate system is defined as the ratio of $R_p$ and $R_s$ (Ref. 2):

$$ \rho = R_p/R_s = \tan\psi \exp(j\Delta), $$

where $\psi$ and $\Delta$ are the two ellipsometric angles measured experimentally.

In the following sections we study the complex-plane representation of the ellipsometric function $\rho$ and its mapping into the real finite $\phi$–$d$ plane. For a given wavelength $\lambda$, we consider $\rho$ as a function of the two main variables $\phi$ and $d$. We end with the presentation of constant-{$\psi$} and constant-{$\Delta$} contours (in the finite $\phi$–$d$ plane) along with their suggested uses in ellipsometry and in the design of reflection-type optical devices, e.g., retarders and polarizers. We take as an example the SiO$_2$–Si film–substrate system at the widely used $\lambda = 6328$-Å He–Ne laser wavelength.

II. Mapping of the Complex $\rho$ Plane onto the $\phi$–$d$ Plane

A. Constant-Thickness Contours (CTC)

When the film thickness $d$ is constant (same sample) and the angle of incidence $\phi$ is changed from 0 to 90°, the ellipsometric function $\rho$ traces a constant-thickness contour [CTC, Fig. 2(a)]. For any film thickness, we have $\rho = -1$ (+1) at $\phi = 0$ (90°). Therefore, these two points are common for all CTCs. For a bare substrate ($d = 0$), we obtain the contour marked $d_0$ in Fig. 2(a) (which coincides with the $-1$ to $+1$ segment of the real axis if the substrate is transparent). As $d$ is increased [e.g., $d = d_1$ in Fig. 2(a)], the CTC moves upward in the upper half of the plane. At a certain value of $d = d_s$, the CTC passes through the point at infinity and consists of two branches, one in the top and the other in the bottom half of the complex $\rho$ plane. Each CTC ($d_0, d_1, \ldots, d_4$) of the complex $\rho$ plane is a horizontal straight line in the $\phi$–$d$ plane (Fig. 2(b)). The portion of the complex $\rho$ plane outside the domain between the $d_0$ and $d_4$ CTCs is the image of the rectangle between the lines $d = d_0$ and $d = d_4$ in the $\phi$–$d$ plane. This leaves the hatched area of the complex $\rho$ plane shown in Fig. 2(a). For $d_4 < d < D_{90}$, say, the CTC is divided into two parts, from $-1$ to $A$ and from $A$ to $+1$ [Fig. 3(a)]. The first part ($-1$ to $A$) lies within the previously mapped...
Fig. 1. Film-substrate system where $N_0$, $N_1$, and $N_2$ are the optical constants of the ambient, film, and substrate, respectively. $\phi$ and $d$ are the angle of incidence of the light beam and the film thickness, respectively.

Fig. 2. (a) Constant-thickness contours (CTCs) in the complex $\rho$ plane for a film-substrate system. (b) CTCs in the reduced angle-of-incidence-film-thickness ($\phi$-$d$) plane.

Section of the complex $\rho$ plane, therefore it intersects with other CTCs. The second part (A to +1) lies within the yet unmapped section of the complex $\rho$ plane. The CTC $d_\rho$ in the $\phi$-$d$ plane is the horizontal line $d_\rho$ shown in Fig. 3(b). Notice that the locus of point A is the CTC $d_0$ in the complex $\rho$ plane and the curve of film-thickness period $D_\rho$ in the $\phi$-$d$ plane. The dashed part of the $d_\rho$ CTC, which intersects with other CTCs, contains no new information and has an image in the reduced $\phi$-$d$ plane $B$-$A'$. The image of the continuous part of the $d_\rho$ CTC is a horizontal line segment in the $\phi$-$d$ plane between $D_\rho$ (point $A$) and the line $\phi = 90^\circ$. It intersects no other CTC. Figure 4(a) shows the complete CTC family of curves in the complex $\rho$ plane that fully covers this infinite plane. Figure 4(b) gives the image of these CTCs in the reduced $\phi$-$d$ plane.

B. Constant-Angle-of-Incidence Contours (CAIC)

We now consider the case when the angle of incidence $\phi$ is constant and the film thickness $d$ is assumed to

Fig. 3. (a) Same as in Fig. 2(a), but for a larger film thickness. (b) CTCs and their images in the reduced $\phi$-$d$ plane.

Fig. 4. (a) Family of CTCs that completely fills the complex $\rho$ plane. (b) The image of the family of CTCs of Fig. 4(a) in the reduced $\phi$-$d$ plane, filling it completely.
Fig. 5. (a) Family of constant-angle-of-incidence contours (CAICs) that completely fills the complex \( \rho \) plane. (b) The image of the family of CAICs of Fig. 5(a) in the reduced \( \Phi-\delta \) plane, filling it completely.

Fig. 6. Families of CTCs and CAICs, superimposed, that completely fill the complex \( \rho \) plane.

Fig. 7. Image of the families of CTCs and CAICs of Fig. 6 in the reduced \( \Phi-\delta \) plane, filling it completely.

change. For a given angle of incidence \( \phi \), the constant-angle-of-incidence contour (CAIC) starts from a point on the bare substrate CTC \( (\delta = 0) \) and \( \rho \) moves in the direction of the arrow as \( \delta \) increases till it reaches the starting point at \( \delta = D_\phi \) [closed contour, (Fig. 5(a)].\(^2\)

If the angle of incidence is increased, we get a larger CAIC that encloses the previous ones and is traversed in the same direction. At a specific angle of incidence \( \phi_s \), the CAIC passes through infinity. For \( \phi > \phi_s \), the corresponding CAIC encloses the point \( \rho = +1 \) (CAIC of \( \phi = 90^\circ \)). For larger angles of incidence, the contours shrink in size to \( 0 \) [+1 point, Fig. 5(a)]. Figure 5(b) shows the CAICs in the \( \Phi-\delta \) plane as vertical straight lines. Figure 6 gives the CAICs and the CTCs superimposed in the complex \( \rho \) plane. Any intersection point \( A \) of a specific value of \( \rho \) is defined by a film thickness \( d \) and an angle of incidence \( \phi \) (two intersecting contours). Figure 7 shows the CAICs and CTCs in the \( \Phi-\delta \) plane as a simple grid of orthogonal straight lines. Now each point in the reduced \( \Phi-\delta \) plane needs to be identified with its corresponding value of \( \rho [= \tan \phi \exp(j\Delta)] \). For this purpose, we introduce the constant-delta and constant-psi contours.

C. Constant-Delta Contours (CDC)

The constant-delta contour (CDC) in the complex \( \rho \) plane is a straight line through the origin making an angle \( \Delta \) with the real axis [Fig. 8(a)]. The image CDC in the \( \Phi-\delta \) plane is shown in Fig. 8(b). In both planes, all CDCs intersect at one point \( P_0 \). At this point, the
film-substrate system functions as a $p$-suppressing polarizer ($\rho = 0$).\textsuperscript{2} The point $P_\infty$ represents the point at infinity where all CDCs intersect once more. At this point, the film-substrate system functions as an $s$-suppressing polarizer ($\rho = \infty$).\textsuperscript{2}

D. Constant-Psi Contours (CPC)

Similarly, the constant-psi contours (CPC) of the complex $\rho$ plane are circles centered at the origin $P_\rho$ of radii equal to $\tan \psi$ [Fig. 9(a)]. Figure 9(b), shows the mapping of those circles onto the $\phi$-$d$ plane, i.e., the CPC of the $\phi$-$d$ plane. All CPCs are closed contours and enclose either $P_0$ or $P_\infty$. Note that the $D_\rho$ line also represents a condition in which the film-coated substrate behaves exactly as the bare substrate and that the two vertical lines at $\phi = 0$ and $90^\circ$ represent the points $-1$ and $+1$ in the complex $\rho$ plane, respectively.

E. Constant-Psi Constant-Delta Contour Maps

Figure 10 shows the CPCs and the CDCs superimposed in the complex $\rho$ plane. The constant-psi constant-delta contour map in the $\phi$-$d$ plane for the SiO$_2$-Si film-substrate system at a $\lambda = 6328$-Å wavelength is shown in Fig. 11.

III. Applications

The constant-psi constant-delta contour maps are very useful in several applications. For example, in laboratory work when one needs a quick estimate of the film thickness from the measured $\psi$ and $\Delta$, the CPC and CDC corresponding to the measured $\psi$ and $\Delta$ are simply identified and their point of intersection gives the required value of $d$. This method can be used by laboratory technicians and requires no knowledge of theoretical ellipsometry.

From this contour map we can get the film thickness $d$ and angle of incidence $\phi$ (for the SiO$_2$-Si film-substrate system at $\lambda = 6328$ Å) for which the system operates as a reflection-type $p$- or $s$-suppressing polarizer,\textsuperscript{2} retarder of any retardation angle,\textsuperscript{3} linear-partial polarizer,\textsuperscript{4} or any reflection-type device of prespecified values of $\psi$ and $\Delta$.\textsuperscript{2} Points $P_0$ and $P_\infty$ correspond to the $p$- and $s$-suppressing polarizers, respectively. The CPC for $\psi = 45^\circ$ gives all possible retarder designs ($\Delta = 0 \rightarrow \pm 180^\circ$). The same contour can be used with the single-element rotating-polarizer ellipsometer (SERPE) to obtain $d$.\textsuperscript{5} The CDC for $\Delta = 0, 180$ gives all possible designs for the linear-partial polarizer. The same contour can be used with polarizer-surface-analyzer (PSA) null ellipsometry to obtain $d$.\textsuperscript{8}
The accuracy of the results obtained by using the maps depends on the accuracy of plotting the map itself and on its size. It is obvious that such a map can easily be generated accurately for any system at any wavelength using a digital computer.

This work was supported by the National Science Foundation grant INT78-00373. This paper was presented, in part, at the 1979 Annual Meeting of the Optical Society of America, Rochester, N.Y.

References

A former president of the International Commission for Optics, Andre Marechal (France) at the ICO-12 meeting in Graz, September 1981.

Photo: W. J. Tomlinson (BTL).