

Analytic inversion of ellipsometric data for an unsupported nonabsorbing uniform layer

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The dielectric constant of a uniform unsupported or embedded layer is shown to satisfy a cubic equation with coefficients determined by the angle of incidence and the measured complex ellipsometric ratio $\rho = r_p/r_s$. Analytic inversion is thus possible. The consequence of measurement errors on the deduced dielectric constant and layer thickness is explored.

INTRODUCTION

One of the main uses of ellipsometry¹ is the determination of the refractive index and thickness of a layer (assumed uniform) by measurement of the ellipsometric ratio $\rho = r_p/r_s$. The usual procedure is numerical.² Here it will be shown that, in the restricted case of an unsupported or embedded uniform layer (the key property needed is that the dielectric constants of the media bounding the film be the same), analytic inversion is possible. The unknown dielectric constant of the layer is shown to satisfy a cubic equation with coefficients determined by the angle of incidence and the measured ellipsometric ratio $\rho = r_p/r_s$, which is variously written as

$$\rho = x + iy = \tan \Psi \exp(i\Delta). \quad (1)$$

CUBIC EQUATION FOR THE DIELECTRIC CONSTANT

The ellipsometric ratio $\rho = r_p/r_s$ for a uniform layer of thickness Δz and dielectric constant ϵ embedded in a medium of dielectric constant ϵ_0 (for example, a film in air) is^{1,3,4}

$$\rho = \frac{p}{s} \frac{1 - s^2 Z}{1 - p^2 Z}, \quad Z \equiv \exp(2iq\Delta z), \quad (2)$$

where s and p are the Fresnel reflection amplitudes of the s and p polarizations:

$$s = \frac{q_0 - q}{q_0 + q}, \quad p = \frac{Q - Q_0}{Q + Q_0}. \quad (3)$$

Here $q_0 = \sqrt{\epsilon_0}(\omega/c)\cos\theta_0$, $q = (\omega/c)(\epsilon - \epsilon_0 \sin^2\theta_0)^{1/2}$, $Q_0 = q_0/\epsilon_0$, $Q = q/\epsilon$, and θ_0 is the angle of incidence. Equation (2) can be solved for Z :

$$Z = \frac{\rho s - p}{ps(\rho p - s)}. \quad (4)$$

Z and thus Δz can be eliminated from the equations if q is real (no absorption in the layer and $\sin^2\theta_0 < \epsilon/\epsilon_0$) because then $ZZ^* = 1$, and thus

$$(\rho s - p)(\rho^* s - p) = p^2 s^2 (\rho p - s)(\rho^* p - s). \quad (5)$$

Equation (5) determines the unknown dielectric constant ϵ in terms of θ_0 and the measured real and imaginary parts of ρ . It will be shown that it reduces to a cubic equation for ϵ/ϵ_0 . First rewrite Eq. (5) in the form

$$|\rho|^2 - (\rho + \rho^*) \frac{p}{s} \frac{1 - (ps)^2}{1 - p^4} + \left(\frac{p}{s}\right)^2 \frac{1 - s^4}{1 - p^4} = 0. \quad (6)$$

From Eqs. (3), we can verify the identities

$$\frac{p}{s} \frac{1 - s^2}{1 - p^2} = 1 - (1 + f)\sin^2\theta_0 \equiv F, \quad (7)$$

$$\frac{p}{s} \frac{1 + s^2}{1 + p^2} = F \frac{1 + f - 2f\sin^2\theta_0}{1 + f - (1 + f^2)\sin^2\theta_0}, \quad (8)$$

$$\frac{2p}{s} \frac{1 - (ps)^2}{1 - p^4} = F \frac{(1 + f)[2 - (1 + f)\sin^2\theta_0]}{1 + f - (1 + f^2)\sin^2\theta_0}, \quad (9)$$

where $f = \epsilon_0/\epsilon$. Note that these identities eliminate the radical $(\epsilon - \epsilon_0 \sin^2\theta_0)^{1/2}$, which appears in the Fresnel reflection amplitudes p and s through q . Substituting into Eq. (6), we find that $f = \epsilon_0/\epsilon$ satisfies a cubic equation, and thus so does $g = \epsilon/\epsilon_0$. This is

$$a_0 + a_1 g + a_2 g^2 + a_3 g^3 = 0. \quad (10)$$

In writing the coefficients a_k , we use the notation

$$\rho = x + iy, \quad \sin^2\theta_0 = \sigma. \quad (11)$$

The coefficients are

$$\begin{aligned} a_0 &= \sigma^2(1 - 2\sigma - x), \\ a_1 &= \sigma[-2 + 7\sigma - 4\sigma^2 + 3x(1 - \sigma) - x^2 - y^2], \\ a_2 &= (1 - \sigma)(1 - 5\sigma + 2\sigma^2) - x(2 - 6\sigma + 3\sigma^2) + x^2 + y^2, \\ a_3 &= (1 - \sigma)[1 - \sigma - x(2 - \sigma) + x^2 + y^2]. \end{aligned} \quad (12)$$

The cubic equation [Eq. (10)] has real coefficients and thus has either one or three real roots; of physical interest are real positive roots. However, we should not throw away complex roots from the start, since (owing to experimental or model errors) the solution relevant to the physical system on which measurements are made may have a small imaginary part.

We thus calculate all three roots for $g = \varepsilon/\varepsilon_0$ by standard techniques⁵: we form the quantities

$$u = (3a_1a_3 - a_2^2)/9a_3^2, \\ v = (9a_1a_2a_3 - 27a_0a_3^2 - 2a_2^3)/54a_3^3 \quad (13)$$

and define w to be one of the roots of $w^2 = u^3 + v^2$. Then in terms of

$$t_1 = (v + w)^{1/3}, \quad t_2 = (v - w)^{1/3}, \quad (14)$$

the values of $g = \varepsilon/\varepsilon_0$ that satisfy Eq. (10) are

$$s - a_2/3a_3, -s/2 - a_2/3a_3 \pm i(\sqrt{3}/2)d, \quad (15)$$

where $s = t_1 + t_2$ and $d = t_1 - t_2$. If $w^2 > 0$, there is one real root. If $w^2 < 0$ (which implies $u < 0$ and $v^2 < -u^3$), there are three real roots, which can be compactly expressed in the trigonometric formula

$$\frac{\varepsilon}{\varepsilon_0} = 2(-u)^{1/2} \cos\left(\frac{\phi + 2\pi m}{3}\right) - \frac{a_2}{3a_3}, \quad (15')$$

where $m = 0, 1, \text{ or } 2$ and $\cos \phi = v/(-u^3)^{1/2}$.

If there are three real values of $\varepsilon/\varepsilon_0$, one must decide among them. Negative roots can be discarded, and usually those with $\varepsilon < \varepsilon_0 \sin^2 \theta_0$ (these correspond to total internal reflection, which can normally be excluded in the present context) can be discarded also. Often two possible values of ε remain, and the choice between them can be made on physical grounds, once the layer thickness has been evaluated from Eq. (4), as follows. In terms of the real and imaginary parts of $\rho = x + iy$, Eq. (4) gives

$$\Delta z = (2q)^{-1} \arctan \frac{y(p^2 - s^2)}{ps(x^2 + y^2) - (p^2 + s^2)x + ps}. \quad (16)$$

Each different value of ε will lead to corresponding values of q and of the Fresnel amplitudes p and s and thus to a different thickness Δz . Multiples of π will, in general, need to be added to the arctangent until a positive and physically reasonable value is obtained. For two or three ε values, two or three pairs of values of ε and Δz can then be compared and the physically most reasonable one selected. For rigorous verification without guesswork, note that a measurement at another angle of incidence or at another wavelength will give other $(\varepsilon, \Delta z)$ pairs, one of which should correspond (within experimental error) to one of the original pairs. Figure 1 shows the inversion of computer-generated data calculated for a layer of refractive index 1.5 ($\varepsilon = 2.25$) and thickness $\omega\Delta z/c = 0.3$ ($\Delta z = 3\lambda_0/20\pi$). We see that the true root for the dielectric constant and its corresponding thickness are steady throughout the angular range, while the nonphysical values are not.

EFFECT OF MEASUREMENT ERRORS

Experimental errors in ellipsometry are usually expressed as errors in Ψ and Δ , where $\rho = x + iy = \tan \Psi \exp(i\Delta)$. In terms of the real and imaginary parts of ρ , errors $\delta\Psi$ and $\delta\Delta$ lead to

$$\delta x = \frac{1 + x^2 + y^2}{(x^2 + y^2)^{1/2}} x \delta\Psi - y \delta\Delta, \\ \delta y = \frac{1 + x^2 + y^2}{(x^2 + y^2)^{1/2}} y \delta\Psi + x \delta\Delta. \quad (17)$$

The currently attainable precision in Ψ and Δ is given as⁶ $\delta\Psi \approx \delta\Delta/2 \approx 1$ mdeg. To demonstrate the effect of errors, we will assume uncertainties of 100 times larger: as much as 0.1 deg in $\delta\Psi$ and $\delta\Delta/2$. Figure 2 shows what the inversion process produces, given a uniform spread of errors in $\delta\Psi$ and $\delta\Delta/2$ about their true (calculated) values and using the same parameters as in Fig. 1.

For an unsupported uniform layer, or more generally, one that is bounded on both sides by media with the same dielectric constant ε_0 , both parts of ρ are zero at the Brewster angle $\theta_B = \arctan(\varepsilon/\varepsilon_0)^{1/2}$. This holds for any thickness Δz of the layer. Thus we expect the thickness to be indeterminate if a measurement is made at the Brewster angle and to be noisy for measurements made near θ_B . Figure 2 shows no indication of such an effect. The reason for this lies in the assumption of $\delta\Psi$ and $\delta\Delta$ as the appropriate error parameters. From Eqs. (17) we can see that near the Brewster angle $\delta x \rightarrow x \delta\Psi/|\rho|$ and $\delta y \rightarrow y \delta\Psi/|\rho|$, with the larger $\delta\Delta$ error contributing nothing at θ_B . Also, near θ_B ,

$$\frac{y}{x} \approx \frac{-s^2 \sin 2q\Delta z}{1 - s^2 \cos 2q\Delta z}, \quad s^2 \approx \left(\frac{\varepsilon - \varepsilon_0}{\varepsilon + \varepsilon_0}\right)^2, \quad (18)$$

so $|y|$ is small compared to $|x|$, thus leading to a small δy at θ_B .

Beaglehole (Ref. 7 and personal communication, D. Beaglehole, Department of Physics, Victoria University of Wellington, New Zealand) believes that a better representation of error, both random and systematic, is obtained by assigning to the real and imaginary parts of ρ independent errors δx and δy . Figure 3 shows the resultant scatter in the values of the dielectric constant and of the thickness found by

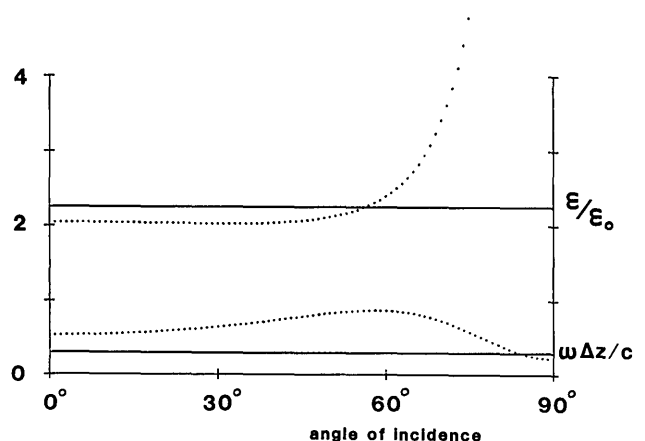


Fig. 1. Inversion of computer-generated values of $\rho = x + iy$ for a uniform layer of dielectric constant 2.25 and thickness parameter $\omega\Delta z/c = 0.3$. In this case there are three real roots of Eq. (10) for $\varepsilon/\varepsilon_0$; one less than $\sin^2 \theta_0$ has been discarded. Of the two remaining, one is nonphysical since it leads to variable ε and Δz (dotted curves). The input values of ε and Δz are reproduced by the other solution (solid lines).

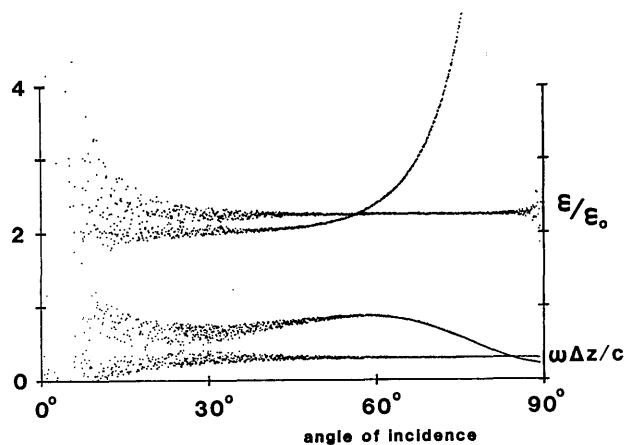


Fig. 2. Scatter in ϵ/ϵ_0 and $\omega\Delta z/c$ values produced by solving Eqs. (10) and (16) if random errors are introduced into the ellipsometric data. Here uniformly distributed errors of up to 0.1° in Ψ and 0.2° in Δ were put in at the start of the inversion process. Note the large scatter near normal incidence.

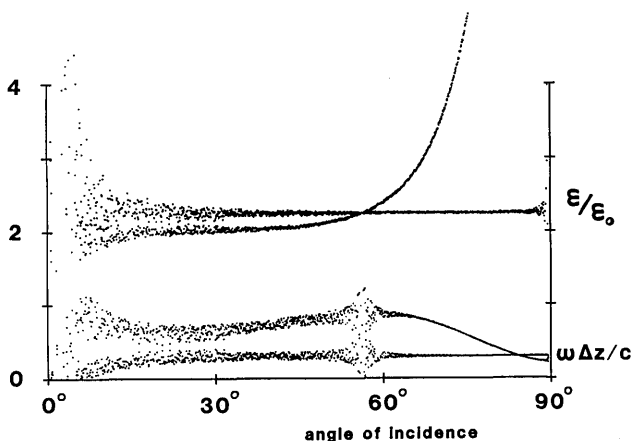


Fig. 3. As for Fig. 2 but with random errors δx and δy (instead of $\delta\Psi$ and $\delta\Delta$), uniformly distributed up to as 0.002.

inversion. Note the large uncertainty near θ_B (56.3°) in the determined thickness. Errors δx and δy approximately 100 times larger than Beaglehole's estimate⁷ of his uncertainty have been used.

DISCUSSION

It has been shown that ellipsometric data can be inverted analytically to find the dielectric constant and thickness of a layer (assumed uniform and nonabsorbing), provided that

the bounding media have the same dielectric constant. A related inversion for an absorbing film is known (Ref. 8 and Sec. 9-2 of Ref. 3); it requires both $\rho = r_p/r_s$ and $\tau = t_p/t_s$, the ratio of the transmission amplitudes.

The more general case (dielectric constants on either side not equal) is as yet unsolved analytically. But we note that it has been shown in Ref. 4 that the thickness can be eliminated from the equations, so that a single equation can be solved for the dielectric constant [Ref. 4, Eq. (34)]. All values of ϵ satisfying this equation are automatically consistent with $Z = \exp(2iq\Delta z)$ being on the unit circle. (This is in contrast to the numerical inversion procedure⁹ in which a value of ϵ is chosen, and the resulting values of Z determined from a quadratic are found, the one closer to the unit circle being chosen to determine the thickness. A nearby value of ϵ gives another value of $|Z|$, and Newton's method gives a better value of ϵ , i.e., with $|Z|$ closer to unity. Iteration then closes in on $|Z| = 1$ numerically.)

In conclusion, it should be noted that with the convention used here, $r_p = r_s$ at normal incidence. The opposite convention has $r_p = -r_s$ at normal incidence, and the consequent change in sign of $\rho = x + iy$. Since the cubic equation [Eq. (10)] has coefficients that depend on x and $x^2 + y^2$, experimenters using the latter convention should change the sign of x in Eqs. (12).

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