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Letter to the Editor

An algorithm for determining the optical constants and thicknesses of thin absorbing layers from the ellipsometric measurements*

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1. Introduction

Ellipsometry in reflected light may be applied to determine the basic parameters of the absorbing layers deposited on an absorbing substrate.

In the paper an algorithm has been presented for determining the complex refractive index ($\tilde{n}_1 = n_1 - ik_1$) and thickness (d) of the absorbing layer deposited on an absorbing substrate of known optical constants (n_2, k_2). The method is reduced to solving the general ellipsometry equation $\tan \Psi e^{\Delta i}$ for this layer system. The programme has been elaborated in Fortran 1900 language, the computations being performed on the Odra 1305 computer.

2. Basic formulae

If the absorbing layer of complex refractive index $\tilde{n}_1 = n_1 - ik_1$ and the thickness d is deposited on an absorbing substrate of the refractive index $\tilde{n}_2 = n_2 - ik_2$, the basic ellipsometry equation for such a system of layers may be written as follows [1–4]:

$$\tilde{\varrho} = \tan \Psi e^{i\Delta} = \frac{\tilde{r}_{1p} + \tilde{r}_{2p} e^{-2i\tilde{\beta}}}{1 + \tilde{r}_{1p}\tilde{r}_{2p} e^{-2i\tilde{\beta}}} \frac{1 + \tilde{r}_{1s}\tilde{r}_{2s} e^{-2i\tilde{\beta}}}{\tilde{r}_{1s} + \tilde{r}_{2s} e^{-2i\tilde{\beta}}}, \tag{1}$$

where

$$\tilde{\beta} = \frac{2\pi}{\lambda} d \sqrt{\tilde{n}_1^2 - n_0^2 \sin^2\varphi_0}, \tag{2}$$

$\tilde{r}_{1p}, \tilde{r}_{2p}, \tilde{r}_{1s}, \tilde{r}_{2s}$ – the Fresnel coefficients for p-and s-components for boundary surfaces of thin layers.

φ_0 – the incidence angle for the light beam.

If we introduce the notation

$$\tilde{\eta} = e^{-2i\tilde{\beta}}, \tag{3}$$

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the equation (1) may be written in the form

$$\tilde{A}\tilde{\eta}^2+\tilde{B}\tilde{\eta}+\tilde{C} = 0 \tag{4}$$

where

$$\tilde{A} = (\tilde{\varrho}\tilde{r}_{1p}-\tilde{r}_{1s})\tilde{r}_{2p}\tilde{r}_{2s}, \tag{5}$$

$$\tilde{B} = (\tilde{\varrho}\tilde{r}_{2s}-\tilde{r}_{2p})+(\tilde{\varrho}\tilde{r}_{2p}-\tilde{r}_{2s})\tilde{r}_{1p}\tilde{r}_{1s}, \tag{6}$$

$$\tilde{C} = \tilde{r}_{1s}\tilde{\varrho}-\tilde{r}_{1p}. \tag{7}$$

After having solved the equation (4) we obtain

$$\tilde{\eta} = -[\tilde{B}\pm(\tilde{B}^2-4\tilde{A}\tilde{C})^{1/2}]/2\tilde{A}. \tag{8}$$

From the formulae (2) and (3) we find the complex thickness of the layer

$$D = \frac{i\lambda}{4\pi}\frac{\ln\tilde{\eta}}{(\tilde{n}_1^2-n_0^2\sin^2\varphi_0)^{1/2}}. \tag{9}$$

Taking account of the fact that only the real part of the thickness has the physical meaning we obtain from (9) the following equations

$$b = \mathrm{Re}\frac{\ln\tilde{\eta}}{(\tilde{n}_1^2-n_0^2\sin^2\varphi_0)^{1/2}} = 0, \tag{10}$$

$$d = \frac{\lambda}{4\pi}\mathrm{Im}\frac{\ln\tilde{\eta}}{(\tilde{n}_1^2-n_0^2\sin^2\varphi_0)^{1/2}}. \tag{11}$$

3. Algorithm

The OPCO programme based on the eqs. (1) and (11) enables to calculate the optical constants n_1 and k_1 and the thickness d of absorbing layers from ellipsometric measurements Δ, Ψ for two different incidence angles (if the optical constants n_2, k_2 of the substrate are known).

For one ellipsometric measurement of Δ, Ψ there exists infinite number of pairs n_1, k_1 each of them corresponding to another thickness of the layer. To chose the proper pair n_1, k_1 another ellipsometric measurement is needed, made, for instance, for another incidence angle. These measurements are denoted by $(\Delta, \Psi)_1$ and $(\Delta, \Psi)_2$.

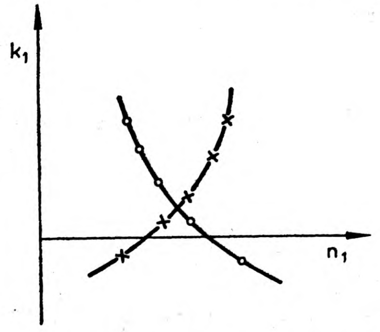
The following data should be introduced to the program:

- n_2, k_2 — optical constants of the substrate,
- Ln_1, Rn_1; Lk_1, Rk_1 — intervals which contain the sought values of n_1 and k_1, respectively,
- Δn_1, Δk_1 — searching sets for intervals of n_1 and k_1, respectively,
- E_b — required accuracy of calculations,
- λ — wavelength,
- $\varphi_0^{(1)}$, $\varphi_0^{(2)}$ — incidence angles,
- Ψ_1, Ψ_2; Δ_1, Δ_2 — experimental values of ellipsometric angles of the system under test.

The necessity to determine the intervals, within which the sought values n_1 and k_1 are surely contained, does not reduce the generality of the programme used, since the intervals may be chosen arbitrarily.

The calculations start with replacing n_1 by the left hand limit Ln_1 of the respective interval and calculating k_1 for $(\Delta, \Psi)_1$. For this purpose the interval Lk_1, Rk_1 is searched by a step Δk_1 to find the root if the eq. (10). Next n_1 is consecutively increased by a step

Δn_1 and for each value of n_1 the respective k_1 is found which satisfies the eq. (10). The above procedure is repeated for $(\Delta, \Psi)_2$. The sequences of pair-values (n_1, k_1) obtained for $(\Delta, \Psi)_1$ and $(\Delta, \Psi)_2$ are stored in the memory. For both the sequences the approximating polynomials w_1 and w_2 are found by the least-square method. The common point of those polynomials determines the sougth value n_1, k_1 (see fig.). In order to find the point of intersection for polynomials the zero-place for a new polynomial $w = w_1 - w_2$ is found. The thickness d of the layer is calculated from the formula (11).



Sequences of n_1, k_1 values obtained for:
$(\Delta, \Psi)_1$ –o–o– and $(\Delta, \Psi)_2$ –×–×–

For each n_1 it is possible to find several values of k_1 which satisfy the eq. (10). In the programme the existence of three values of k_1 is forseen for each n_1, and consequently three curves may be obtained for both $(\Delta, \Psi)_1$ and $(\Delta, \Psi)_2$. Practically, the number of curves is less than 3, since for any n_1 more than one value of k_1 is seldom obtained. The best solution of those generated by the computer has to be found as a next step of processing. In most cases many solutions are obtained even from the intersection of two curves, since the approximating polynomial in the OPCO programme may be of second to fifth degree (depending on the number of measurement points). All the solutions lying outside the given intervals for n_1 and k_1 are rejected. The optimal solution is assumed to be such for which the error E, calculated as a sum of absolute values of differences between the angles Δ and Ψ obtained experimentally and calculated from the found values of n_1, k_1 and d, is minimum.

A simplified scheme of the OPCO programme was reported in [5]. The following subroutines were employed in the OPCO programme:

RTMI [6] – which determines the root of nonlinear equation $f(x) = 0$ by the Mueller iteration method,

CPOLY [7] – subroutine determining all the zeros of the complex polynomial,

FREGREPARAB [8] – which determines the parabolic regression coeff cients of k-th degree of the form $y = b_1 + b_2x + \ldots + b_{k+1}x^k$.

4. Results

The elaborated programme has been verified for a number of tabularized values reported in the paper [9] for a system SiO_2 on Si (table).

Verification of calculation correctness

	n	k	d [nm]	E
Tabelarized values	1.41	0	100	–
Calculated	1.4094	0.00039	100.09	0.0059

The analysis of the OPCO programme indicates that it may be applied to calculate the optical constants and the thicknesses of absorbing layers not thicker than 40 nm and deposited on the substrates of known optical constants.

The OPCO programme was employed to determine the optical constants and thicknesses of thin chromium oxide layers deposited on the chromium substrate with the help of an electron gun. The ellipsometric angles corresponding to different thicknesses of Cr_2O_3 on Cr layers were measured within the visible spectral region (450–650 nm) for two angles of incidence (65° and 70°).

The examinations have shown that the oxide layers of thicknesses $d < 70$ nm in the visible range exhibit a constant value of the complex refractive index

$$\tilde{n} = (2.00 \pm 0.03) - i(0.02 \pm 0.01).$$

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