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Letter to the Editor

An algorithm for determining the refractive index and thickness of thin dielectric layers on an absorbing substrate on the basis of ellipsometric measurements

Elżbieta Idczak, Ewa Oleszkiewicz, Krystyna Żukowska

Institute of Physics, Technical University of Wrocław, Wrocław, Poland.

Introduction

An all the applications of ellipsometry an interpretation of directly measured quantities, i.e. of the so-called ellipsometric angles Δ and Ψ consists in a transition to optical constants of the substrate (n_3, k_3), optical constants (n_2, k_2) and thickness (d) of the upper layer. From the mathematical viewpoint this means the solving of the general equation of ellipsometry $\tan \Psi e^{i\Delta}$ for a substrate — thin film system. This equation can not be solved explicite with respect to n_2, k_2 and d, therefore it is solved either by graphic methods or by using simplified formulae.

In this work an algorithm has been developed for determining the refractive index (n_2) and the thickness (d) of the dielectric layer on the absorbing substrate of known optical constants (n_3, k_3).

The respective program in Fortran IV has been elaborated for R-32 computer. This program may work under DOS/JS or OS/JS system control.

Basic relations

If a dielectric layer of refractive index (n_2) and thickness (d) is deposited on an absorbing substrate (n_3, k_3), then the basic equation of ellipsometry for such a system may be written down as follows [1–3]:

$$\tan \Psi e^{i\Delta} = \tan \overline{\Psi} e^{i\overline{\Delta}} \frac{(1+cP)(1+gP)}{(1+eP)(1+fP)} \tag{1}$$

where $\overline{\Delta}$ and $\overline{\Psi}$ are the ellipsometric angles for the substrate applied, i.e.

$$\tan \overline{\Delta} = \frac{2hn_1 \sin\varphi_1 \tan\varphi_1}{n_1^2 \sin^2\varphi_1 \tan^2\varphi_1 - h^2 - l^2}, \tag{2}$$

$$\tan 2\overline{\Psi} = \frac{h}{l \sin \overline{\Delta}}, \tag{3}$$

$$\left.\begin{matrix} h \\ l \end{matrix}\right\} = \{\mp 1/2 (n_3^2 - k_3^2 - n_1^2 \sin^2\varphi_1) + 1/2 [(n_3^2 - k_3^2 - n_1^2 \sin^2\varphi_1)^2 + 4n_3^2 k_3^2]^{1/2}\}^{1/2}, \tag{4}$$

$$P = \tan h \left(\frac{i2\pi}{\lambda} d n_2 \cos\varphi_2\right), \tag{5}$$

$$\left.\begin{matrix} c \\ e \end{matrix}\right\} = \frac{n_1 \cos\varphi_1}{(n_3 - ik_3)\cos\varphi_1 \mp n_1 \cos\varphi_3} \left[\frac{n_2 \cos\varphi_3}{n_1 \cos\varphi_2} \mp \frac{(n_3 - ik_3)\cos\varphi_2}{n_2 \cos\varphi_1}\right], \tag{6}$$

$$\left.\begin{matrix} f \\ g \end{matrix}\right\} = \frac{n_1 \cos\varphi_1}{n_1 \cos\varphi_1 \mp (n_3 - ik_3)\cos\varphi_3} \left[\frac{(n_3 - ik_3)\cos\varphi_3}{n_2 \cos\varphi_2} \mp \frac{n_2 \cos\varphi_2}{n_1 \cos\varphi_1}\right], \tag{7}$$

$$n_1 \sin\varphi_1 = n_2 \sin\varphi_2 = (n_3 - ik_3)\sin\varphi_3. \tag{8}$$

To simplify the calculation it is convenient to introduce the following quantity

$$z = \frac{\tan\Psi e^{i\Delta}}{\tan\overline{\Psi} e^{i\overline{\Delta}}} = \frac{(1+cP)(1+gP)}{(1+eP)(1+fP)}. \tag{9}$$

The solution of equation (9) with respect to P gives

$$P = \frac{-[(c+g)-(f+e)z] \pm \{[(c+g)-(f+e)z]^2 + 4(z-1)(cg-efz)\}^{1/2}}{2(cg-efz)}. \tag{10}$$

The elaborated algorithm requires the measurement of ellipsometric angles Δ and Ψ for a layer-absorbing substrate system with a given angle of incident φ_1, wavelength λ, and the knowledge of optical constants (n_3, k_3) or ellipsometric angles $(\overline{\Delta}, \overline{\Psi})$ of the substrate used.

Algorithm

Solution of equation (1) is reduced to solving the following equations:

$$d = f_1(n_2, n_3, k_3, n_1, \Delta_{\text{exp}}, \Psi_{\text{exp}}, \varphi_1, \lambda), \tag{11}$$

$$\Delta_{\text{calc}} = f_2(n_1, n_2, \text{Re}(d), n_3, k_3, \varphi_1, \lambda), \tag{12}$$

$$\Psi_{\text{calc}} = f_3(n_1, n_2, \text{Re}(d), n_3, k_3, \varphi_1, \lambda), \tag{13}$$

where:

$\Delta_{\text{exp}}, \Psi_{\text{exp}}$ – experimental values of the examined system,
$\Delta_{\text{calc}}, \Psi_{\text{calc}}$ – values of Δ and Ψ to be calculated,
$n_1, n_3, k_3, \varphi_1, \lambda$ – are considered as parameters.

Given the region of change of $n_2 \in N$ the values $d_j = f_1(n_{2j})$ for which $\text{Im}(d_j) \simeq 0$ are also sought.

Next for those values $d_j \in D$ the function

$$B(n_{2j}) = \sqrt{\left|\frac{\text{Re}(d)-\text{Im}(d)}{\text{Re}(d)}\right|^2 + \left|\frac{\Delta_{\text{exp}}-\Delta_{\text{calc}}}{\Delta_{\text{exp}}}\right|^2 + \left|\frac{\Psi_{\text{exp}}-\Psi_{\text{calc}}}{\Psi_{\text{exp}}}\right|^2} \tag{14}$$

is determined and its minimum is sought. The solutions of the equation (1) are given by the $n_{2\,\text{opt}}$, for which $B(n_{2\,\text{opt}}) = \min$ and $d_{\text{opt}} = f_1(n_{2\,\text{opt}})$ at the given parameters. A simplified algorithm is presented in figure.

Besides the given quantities $\Delta_{\text{exp}}, \Psi_{\text{exp}}, n_3, k_3, n_1, \varphi_1, \lambda$ we define also the variability range for $n_2\,(n_{2\,\text{max}} - n_{2\,\text{min}})$, in which the sought solution should be expected. The layer thickness d_j is calculated from the formulae (5), (9) and (10) for all the quantities

$$n_{2j} = n_{2\,\text{min}} + (j-1)\Delta n_2, \quad j = 1, \dots, m,$$

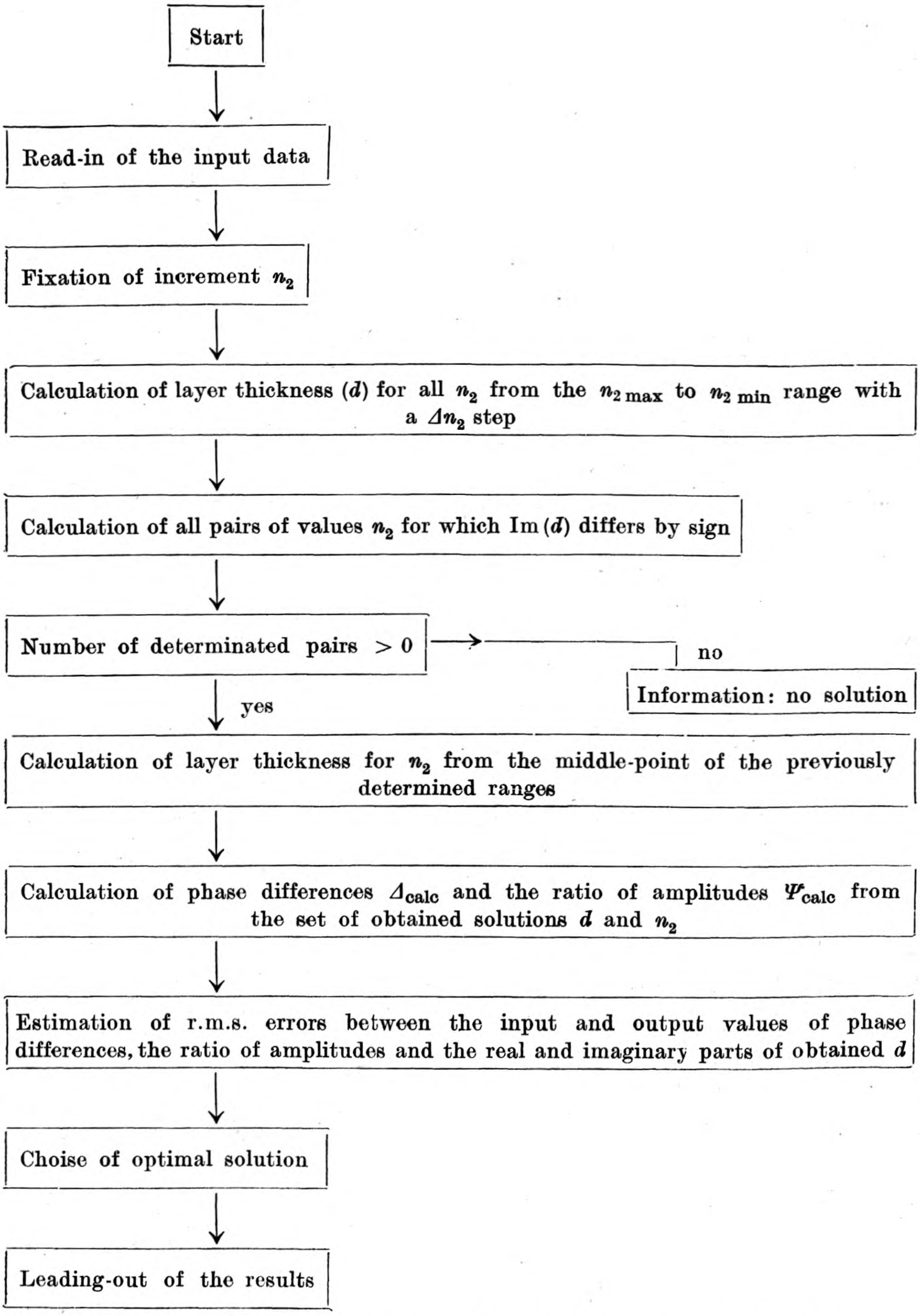
where

$$m = \frac{n_{2\,\text{max}} - n_{2\,\text{min}}}{\Delta n_2}$$

and

$$\Delta n_2 = 0.01.$$

Since the required solution should be real from all the complex values of d_j we must accept such for which $\text{Im}(d_j) \simeq 0$. The choise is made by analysing the function $\text{Im}(d_j) = f_4(n_{2j})$. All the values of n_2 for which $f_4(n_{2j})$ changes its sign are kept in the memory of the computer. If the solution exists then it should be found among the obtained values of n_{2j}. Next from the formulae (1)–(8) we calculate the values of $\Delta_{\text{calc}}, \Psi_{\text{calc}}$ and the differences $|\Delta_{\text{calc}} - \Delta_{\text{exp}}|$, $|\Psi_{\text{calc}} - \Psi_{\text{exp}}|$, the rms. error from



the formula (14), assuming that the values of φ_1, λ, n_1, n_3, k_3 as well as those of n_{2j} and $\mathrm{Re}(d_j)$ obtained from calculations, are input data. The values of n_{2j} and $\mathrm{Re}(d_j)$, for which the r.m.s. error is minimal are considered to be an optimal solution. The equation (1) may either give several optimal solutions or for some pairs of values of Δ_{exp},

$\Psi_{\exp}$ no solution at all, since the quantities $\Delta_{\exp}$ and $\Psi_{\exp}$ suffer always from measuremental errors. If there exist several solutions then the choise of proper (n_2, d) pairs may be made by analysing the equation (1) for the same layer at different wavelengths or at different angles of incidence φ_1. If, however, the equation has no solution the program generates new values of $\Delta_{\exp} \pm \delta\Delta$, $\Psi_{\exp} \pm \delta\Psi$ and optimal solutions of equation (1) are sought for all combinations of these quantities.

The results

The algorithm proposed has been verified for a number of tabularised values taken from the work by GERGELY [4] given for a system SiO_2 on Si. Some results of calculations have been presented in table. The consistency of the results should be considered satisfactory.

Input data
Substrate parameters $N = 3.85$, $K = 0.02$

Angle of incident	Δ	Ψ	Wave-length
70.0	227.180	79.043	623.8 nm
	275.116	43.781	
	162.921	10.668	

Range of $N_2(N_{2\,\max} - N_{2\,\min})$ 3.00 – 1.00 $K2 = 0$
Optimal values

EN3	PK3	END WA	PK2	ZED		Ψ	ΨUW	Δ	ΔUW
3.85	0.02	1.41	0.0	155.001	0.002	79.04	79.03	227.18	227.11
3.85	0.02	1.41	0.0	190.002	0.004	43.78	43.47	275.11	275.07
3.85	0.02	1.41	0.0	6.145	−0.002	10.66	10.40	162.92	162.55

The analysis of calculation accuracy of n_2 and d has shown that the refractive index is calculated with the accuracy ± 0.01 while the accuracy of the dielectric layers thickness determination amounts to ± 0.1 nm.

Because of the type operations performed in the program the lower range of the original data region of $n_2 \in N$ must differ from zero. The computing time is directly proportional to the area of N region.

References

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[3] GORSHKOV M. M., Ellipsometriya, Sovetskoe Radio, Moskva 1974.
[4] GERGELY G., *Ellipsometric Tables of the Si – SiO$_2$ System for Mercury and HeNe Laser Spectral Lines*, Académiai Kiadó, Budapest 1971.

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Anouncement

The VII th International Congress
"Intercamera"
will be held on 21–22 March 1979 at the Hotel Intercontinental in Prague, Czechoslovakia. The general topic will be "Optoelectronic Applications in Audiovisual Technique.
The Technical Salon "Intercamera" will be inaugurated at the same time with the participation of more than 100 foreigen manufactures.