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Modelling of the thin-film structure for the purpose of ellipsometric measurements

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A method of designing an optical model of a layer structure by fitting the calculated characteristics to the characteristics obtained from measurements of the ellipsometric angles Ψ and Δ of a real sample is presented in the paper. An example of an application of the program as well as the procedures of fitting for a thin natural layer on the surface of a silicon substrate are demonstrated.

1. Introduction

Ellipsometry is one of the research methods that allows us to obtain information about structural, optical and electronic characteristics of a wide range of materials. It is an optical method and it does not damage investigated structures. It is based on an analysis of the change of the incident light polarization state, which is the result of either reflection or transmission. High sensitivity of the method allows detection of extremely thin layers placed on any structure. The main applications of the ellipsometric method are:

– describing optical characteristics of an investigated material,
– describing optical characteristics and thickness of thin films,
– analysis of the composition and geometry of one-layer structures,
– investigating the profile of the additive distribution in a semi-conducting material.

Realization of the above mentioned tasks is possible thanks to the analysis of ellipsometric parameters obtained in experiments in comparison with ellipsometric parameters calculated theoretically, having an assumed optical model of the examined structure [1], [2].

2. Theory and calculations

To provide a definition of ellipsometric parameters, we can start with the electromagnetic theory of light. By solving Maxwell equations we get the following expression on an electrical field vector $\boldsymbol{E}$ of a plane wave moving in a medium:

$$\boldsymbol{E} = \boldsymbol{E}_0 \exp j(\omega t - N\boldsymbol{\varkappa}\boldsymbol{r}) \tag{1}$$

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where: $\boldsymbol{E}_0$ – stands for both an amplitude and direction of the polarization of the wave in relation to the incident plain, ω – an angular frequency, t – time, $N = n - jk$ – complex refraction index of a medium, n – refraction index, k – extinction index, $\boldsymbol{\varkappa}$ – wave vector, $\boldsymbol{r}$ – direction of propagation.

An incident electrical field vector $\boldsymbol{E}$ falling on the border between two media can be divided into two components: parallel (p) and perpendicular (s) to the incident plain $\boldsymbol{E} = \boldsymbol{E}_{\text{inc}} = \boldsymbol{E}^{\text{p}}_{\text{inc}} + \boldsymbol{E}^{\text{s}}_{\text{inc}}$. Analogically, an electrical field vector reflected from the border between two media, or refracted on it, has two components (p and s). The ratio of the polarized components (p and s) of electrical field vectors: a refracted one to an incident one is described by Fresnel complex coefficient

$$\frac{\boldsymbol{E}^{\text{p}}_{\text{ref}}}{\boldsymbol{E}^{\text{p}}_{\text{inc}}} = r^{\text{p}}, \quad \frac{\boldsymbol{E}^{\text{s}}_{\text{ref}}}{\boldsymbol{E}^{\text{s}}_{\text{inc}}} = r^{\text{s}}. \tag{2}$$

By substituting proper expressions obtained from solving Maxwell equations into the above formulas and considering an edge condition (continuity of tangent components $\boldsymbol{E}$ and $\boldsymbol{H}$ at the crossing of the border between the media 0 and 1), we get:

$$r^{\text{p}} = \frac{N_1 \cos\Phi_0 - N_0 \cos\Phi_1}{N_1 \cos\Phi_0 + N_0 \cos\Phi_1}, \quad r^{\text{s}} = \frac{N_0 \cos\Phi_0 - N_1 \cos\Phi_1}{N_0 \cos\Phi_0 + N_1 \cos\Phi_1} \tag{3}$$

where N_0 and N_1 stand for refraction indexes of the media 0 and 1, respectively (N_1 complex), and Φ_0 and Φ_1 for the incident angle in medium 0 and the refraction angle in medium 1 (Φ_1 complex). When we write Fresnel coefficients as:

$$r^{\text{p}} = |r^{\text{p}}|\exp(j\delta_{\text{p}}) \text{ and } r^{\text{s}} = |r^{\text{s}}|\exp(j\delta_{\text{s}}), \tag{4}$$

and divide both sides by themselves, we get Drude equation

$$\frac{r^{\text{p}}}{r^{\text{s}}} = \frac{|r^{\text{p}}|}{|r^{\text{s}}|}\exp j(\delta_{\text{p}} - \delta_{\text{s}}) = \tan\Psi \exp(j\Delta) = \rho. \tag{5}$$

Parameters Ψ and Δ introduced into the above formula are called ellipsometric angles. They represent the change of amplitudes and component phases (p) and (s) of an electrical field vector of an incident wave, which takes place as a result of the reflection from the border between two media. Formula (5), called Drude equation, relates value ρ (by Fresnel coefficient) to the values of the angle of incidence and the refraction indexes of media 0 and 1, which can be written symbolically as (a zero-layer model of optical structure):

$$\rho = \tan\Psi \exp(j\Delta) = \rho(N_0, N_1, \Phi_0, \lambda) \tag{6}$$

or

$$\Psi = \Psi(N_0, N_1, \Phi_0, \lambda), \quad \Delta = \Delta(N_0, N_1, \Phi_0, \lambda). \tag{7}$$

In the case where a light wave falls on a medium having a multilayer structure with p layers (substrate index p+1), with different values of refraction index and different thickness values for particular layers d formula (7) changes into:

$$\rho = \tan\Psi\exp(j\Delta) = \rho(N_0, N_1, \ldots, N_p, N_{p+1}, d_1, \ldots d_p, \Phi_0, \lambda) \tag{8}$$

or

$$\Psi = \Psi(N_0, N_1, \ldots, N_p, N_{p+1}, d_1, \ldots, d_p, \Phi_0, \lambda),$$
$$\Delta = \Delta(N_0, N_1, \ldots, N_p, N_{p+1}, d_1, \ldots, d_p, \Phi_0, \lambda). \tag{9}$$

Ellipsometric parameters Ψ and Δ are the functions of the optical characteristics of a structure, angle of incidence Φ and light wave length λ. As a result of this, we have the possibility of distinguishing the following kinds of ellipsometric methods:

– monochromatic ellipsometry: measurement of ρ with $\lambda = \text{const}$ and one variable, *e.g.*, an angle of incidence or thickness of a layer,

– spectroscopic ellipsometry: measurement of ρ as a function of λ,

– kinetic ellipsometry: measurement of ρ as a function of time,

– spatial ellipsometry: measurement of ρ as a function of the location of a measurement point on a measured structure.

Parameters Ψ and Δ can be calculated with the help of the above mentioned relationships. On the other hand, they can be measured by an ellipsometer. Comparing the measured pair Ψ, Δ with the calculated pair Ψ, Δ, we can determine the values of the two parameters, *e.g.*, n_1 and d_1, by asigning an optical model assumed for calculations to a real structure. This very simplified procedure is often applied. The assumed model does not always reflect the complexity of an investigated structure. Thus, it is advisable to treat each investigated structure individually and to work out its optical model.

Working out the model of an investigated structure consists in finding a distribution of the refraction index as a function of depth such that calculated ellipsometric functions, *e.g.*, $\Psi(\Phi_0)$, $\Delta(\Phi_0)$ – for monochromatic ellipsometry or $\Psi(\lambda)$, $\Delta(\lambda)$ – for spectroscopic ellipsometry be consistent with analogical measured ellipsometric functions. In order to do so we need:

1. A program for calculating ellipsometric angles of a model structure with unrestricted distribution of optical parameters.
2. Methodology of procedures and calculations, whose aim is to fit the model structure to the real structure.

With an assumption that any real structure can be approximated by a multilayer structure with constant values of refraction index in particular layers, a program for calculating ellipsometric angles was based on a recursion process of calculating admittance $Y_m = H_m/E_m$ for successive borders between the layers beginning with the border between the substrate (index p+1) and the last layer (index p) – Y_p, and ending with the border between the first layer (index 1) and the immersion medium (index 0) – Y_0, [3]. The general form of the recursion formula for the admittance of a successive transition is as follows:

$$Y_{e,m-1} = a_{m-1} + jb_{m-1} = \frac{Y_{e,m}\cos D_{e,m} + jN_{e,m}\sin D_{e,m}}{\cos D_{e,m} + j\,Y_{e,m}\sin D_{e,m}/N_{e,m}}, \tag{10}$$

where index e is an effective value of a certain parameter, index m – a number of the border between layers m and m+1, $D_{e,m} = (2\pi/\lambda)N_{e,m}d_m\cos\Phi_m$ – complex effective phase thickness of layer m, Φ_m – refractive angle in the m-th layer calculated from Snell law. An initial condition of the process of admittance calculation is admittance Y_p between the substrate and the layer p. The admittance Y_p equals

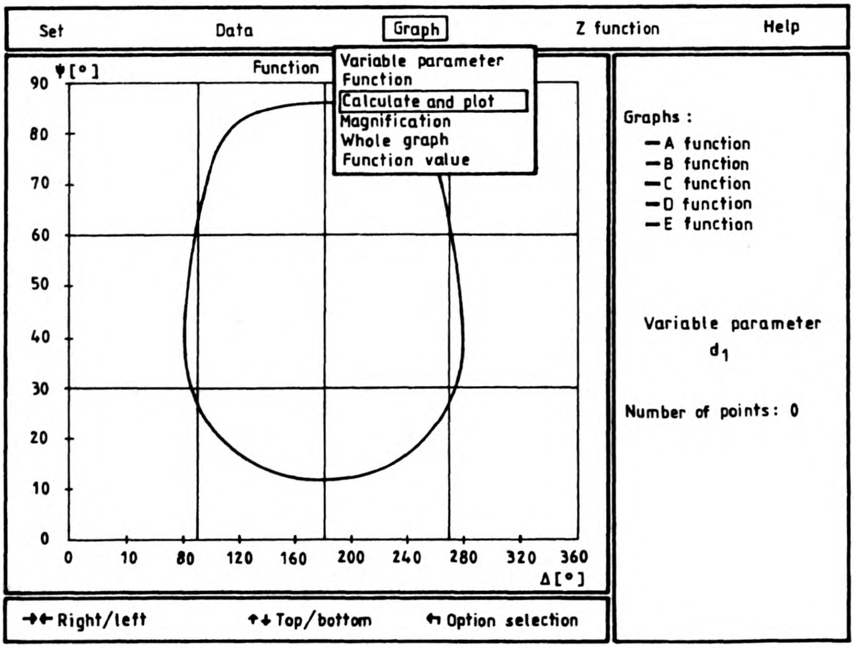
$$Y_p = N_{p+1} = n_{p+1} - jk_{p+1}. \tag{11}$$

On the basis of the calculated admittance Y_0, we calculate the reflection index for polarization (p) and (s) from the formula

$$r^{p,s} = \frac{N_0 - Y_0^{p,s}}{N_0 + Y_0^{p,s}}. \tag{12}$$

Then we calculate ellipsometric parameters from Drude formula.

The prepared program [4] allows calculation and presentation in the form of graphs or tables, of the ellipsometric angles Ψ, Δ as a function of one of the parameters for an optical model with not more than 20 layers. It is possible to present six functions – five calculated, each for a different set of parameters, corresponding to the different model structures, and one measured. The program allows analysis of the changes of calculated ellipsometric angles as a function of any parameter. Calculated functions are presented graphically on the monitor screen. The possibility of enlarging any fragment of the graph significantly increases accuracy of the presented picture. The applied system of resizable, multiple windows, an ease of changing the structure of a model as well as changing any parameters, the choice of calculating and graphing any function make the program user-friendly (Fig. 1).



Variable parameter d_1

Number of points: 0

Fig. 1. Graphic representation of an ellipsometric function on the computer monitor

The methodology of procedures, whose aim is to fit a model to the real structure, is based on the criterion of an error defined as a sum $(\Psi_{\mathrm{meas}}-\Psi_{\mathrm{calc}})+(\Delta_{\mathrm{meas}}-\Delta_{\mathrm{calc}})$. The process of fitting begins with the assumption of the simplest model, which can be accepted for a given structure. Then moving from the border "immersion medium – surface of an investigated structure", and modifying particular optical parameters as well as the structure of an assumed model, by successive iterations, we should reach such a stage of fitting that the divergence between the theoretical and the experimental curves be within the limits of a measurement error. Each step in the process of fitting is a change of one parameter only and analysis of one of the ellipsometric functions Ψ or Δ.

3. Conclusions

Modelling processes for silicon substrates are presented in Figures 2 and 3. Experimental data are marked with crosses, while theoretical graphs are represented by solid lines. An assumption of the homogeneity of a silicon substrate with constant values of refraction indices 4.05 and extinction indices 0.028 does not reflect reality.

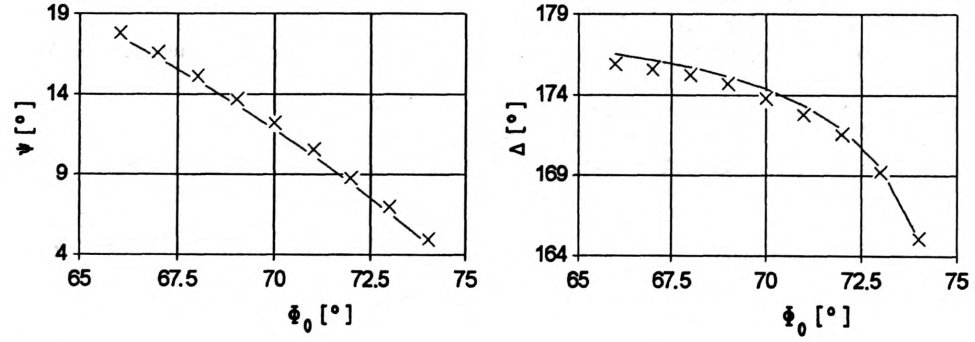


Fig. 2. Functions $\Psi(\Phi_0)$ and $\Delta(\Phi_0)$: calculated (solid lines) and experimental ones at the moment of beginning of the modelling process

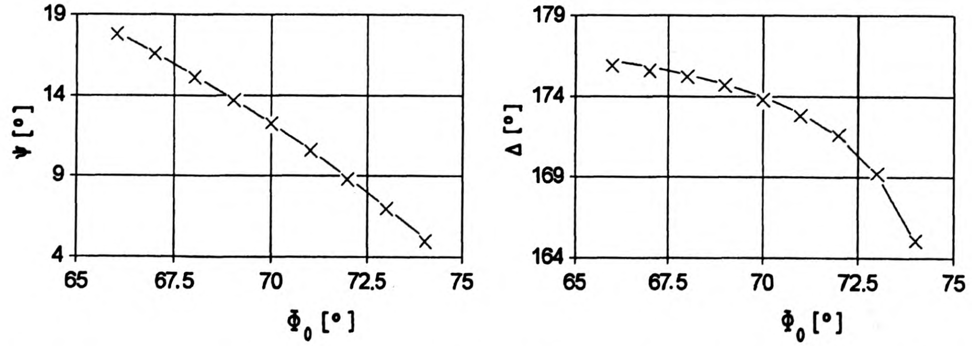


Fig. 3. Functions $\Psi(\Phi_0)$ and $\Delta(\Phi_0)$: calculated (solid lines) and experimental ones after finishing the modelling process

It follows from the measurements that on the surface of the substrate there is a layer whose optical parameters are different from those of silicon. The existence of this layer is physically justified by technological processes the substrate was exposed to. Using the prepared method of computer modelling of the layer structures, an optical model was fitted to an investigated substrate and the results are shown in Fig. 3. Lines on the graphs $\Psi(\Phi_0)$ and $\Delta(\Phi_0)$ calculated and measured overlap and the divergence between the corresponding points is within the limits of a measurement error. It follows from the measurements that the following optical model can be assigned to the investigated substrate:

first layer	$n_1 = 1.46$	$k_1 = 0.000$	$d_1 = 1.5$ nm
second layer	$n_2 = 4.06$	$k_2 = 0.050$	$d_2 = 2.0$ nm
third layer	$n_3 = 4.08$	$k_3 = 0.055$	$d_3 = 7.0$ nm
fourth layer	$n_4 = 4.05$	$k_4 = 0.038$	$d_4 = 15.0$ nm
substrate	$n_p = 4.05$	$k_p = 0.028$	

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