OPTICAL METHODS FOR ANALYSIS OF THIN DIELECTRIC FILMS

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1. Introduction

Fundamental quantity for description of the the optical response of material, represented by the polarization $\boldsymbol{P}$, is the electric susceptibility χ_e. It gives the relation between the intensity of electric field $\boldsymbol{E}$ and the polarisation of material $\boldsymbol{P}$

$$\boldsymbol{P} = \chi_e \varepsilon_0 \boldsymbol{E} = \left(\varepsilon_r - 1\right)\varepsilon_0 \boldsymbol{E}. \tag{1}$$

Very often the dielectric function $\varepsilon_r = \chi_e + 1$ is used instead of the electric susceptibility. The dielectric function is a complex quantity, the imaginary part describes the phase shift of the displacement $\boldsymbol{D}$ and $\boldsymbol{E}$ in lossy materials and in general it is a tensor quantity, used for the description of properties of anisotropic materials.

For the description of optical response of various materials the dielectric function model $\varepsilon_r(\omega)$ can be created. The basic $\varepsilon_r(\omega)$ model is derived from a classical oscillator model in which the system of electrons shows the resonance at angular frequaency ω_0

$$\varepsilon_r(\omega) = 1 - \frac{\omega_p^2}{\omega^2 - \omega_0^2 + i\omega\gamma}, \tag{2}$$

where ω_p is the collective resnance frequency of the electrons and γ is a phenomenological Lorenzian line broadening parameter. In reality several different transitions ω_j are possible and Eq.(2) can be generalized to

$$\varepsilon_r(\omega) = \varepsilon_\infty - \omega_p^2 \sum_j \frac{f_j}{\omega^2 - \omega_j^2 + i\omega\gamma_j}, \tag{3}$$

where f_j is the oscillator strength and ε_∞ represents all resonances at frequencies higher than the experimental limit [1].

Based on the Lorentz model of the dielectric function the spectral reflectance R can be determined and used for the interpretation of the reflectance experiment. Similarly the ellipsometric parameters (Ψ, Δ) can be computed and used in a construction of the theoretical model for the ellipsometric experiment, providing the complex reflection ratio

$$\rho = \tan\Psi \exp(i\Delta) \tag{4}$$

values for defined experimental frequencies ω_i [2].

2. Experimental methods

In our approach the theoretical model is constructed by using computer simulation in visual graphic environment followed by the stochastic optimization based on the genetic algorithm and finally refined by suitable gradient optimization method (Levenberg-Marquardt method) [3]. The theoretical model contains also information about the material and structure inhomogeneities incorporated by introduction of the effective media approximation models.

Results of the optimized theoretical models for the spectral reflectance and ellipsometric experiments are used for the determination of the optical responses of given materials and geometrical properties of the layered structure. Analysis of optical properties performed by this method provides reliable results that can be used for characterization of the development of material properties under the physical treatment operations. The analytical procedure is laborious and time-consuming. For the evaluation of specific parameter, for example the thickness of the thin film t_f on a thick substrate, faster methods can be used. In the next section we shall describe such methods for the determination of t_f from the spectral reflectance as well as from the ellipsometric data.

2.1. Analytical methods for fast determination of the film thickness

Light reflected from the top and bottom of the film interfaces interferes and creates fringes in the spectral reflectance pattern. An interference maximum appears at wavelength λ satisfying equation

$$t n_1 \cos\theta_1 = (2m+1)\frac{\lambda}{4},\ m=0,1,2,... \tag{5}$$

where n_1 is the refractive index of the film, θ_1 is the refraction angle in the film [4]. Interference minima result from equation

$$t n_1 \cos\theta_1 = 2m\frac{\lambda}{4}. \tag{6}$$

From Eq.(5) and (6) we can see that the distance between the maximum and next minimum in the reflectance pattern is $\lambda/4$. Using this information the *m* values can be assigned to the observed reflectance extrems. The film thickness is then determined by using proper $m, n_1(\lambda)$ and θ_1 values.

For the reflectance function with sufficient amount of interference fringes the power spectral density PSD [5] of the reflectance function can be used to dermine the film thickness. The idea is based on the analogy between properties of periodic functions and their spectral analysis. Instead of the signal frequency the "space frequency" directly connected with the film thickness is obtained. The PSD of the reflectance function *R* shows peak at the film thickness *t* position.

In the thin film/substrate structure the complex reflection ratio $\rho = \frac{P^\pi}{P^\sigma}$ is determined by the π and σ components of the total reflection coefficients *P* of polarized light. Reflection coefficients P are computed by using Fresnel reflection coefficients $r_{ij}^{\pi,\sigma}$, defined for given interface $ij = 01,12$ and polarization component π, σ

$$\rho = \frac{\left(r_{01}^{\pi} + r_{12}^{\pi} e^{-i2\beta}\right)\left(1 + r_{01}^{\sigma} r_{12}^{\sigma} e^{-i2\beta}\right)}{\left(1 + r_{01}^{\pi} r_{12}^{\pi} e^{-i2\beta}\right)\left(r_{01}^{\sigma} + r_{12}^{\sigma} e^{-i2\beta}\right)}, \tag{7}$$

where $\beta = \dfrac{2\pi t}{\lambda}\sqrt{n_1^2 - n_0^2 \sin^2 \theta_0}$, t is the film thickness, λ is the wavelength of incident light, n_i is complex refractive index of corresponding media i and θ_0 is angle of incidence [6]. In the spectral ellipsometry experiment the complex reflection ratio ρ is described by the ellipsometric parameters (Ψ, Δ) obtained from the measurement according Eq.(4). By combining Eq.(7) and (4) we obtain complex equation

$$\tan\Psi \exp(i\Delta) = \frac{a_2 x^2 + a_1 x + a_0}{b_2 x^2 + b_1 x + b_0} \tag{8}$$

where $a_0 = r_{01}^p$, $a_1 = r_{01}^p r_{01}^s r_{12}^s + r_{12}^p$, $a_2 = r_{12}^p r_{01}^s r_{12}^s$, $b_0 = r_{01}^s$, $b_1 = r_{01}^p r_{12}^p r_{01}^s + r_{12}^s$, $b_2 = r_{01}^p r_{12}^p r_{12}^s$, $x = e^{-i2\beta}$,
in which two ellipsometric parameters Ψ and Δ are related to the complex refractive indices, the angle of incidence, the wavelength and the film thickness. The film thickness can be determined by using a solution x of Eq.(8)

$$t = \frac{i\lambda \ln x}{4\pi\sqrt{n_1^2 - n_0^2 \sin^2 \theta}}. \tag{9}$$

3. Results and discussion

Results from the theoretical modeling of the spectral reflectance of amorphous hydrogenated silicon samples on glass are shown in Fig. 1. The spectral reflectance pattern changes with the hydrogen dilution parameter D during the plasma PECVD deposition of Si. By computing of the reflectance function with the Lorenzian model Eq.(3) a good quality of theoretical model can be achieved (Fig. 1b).

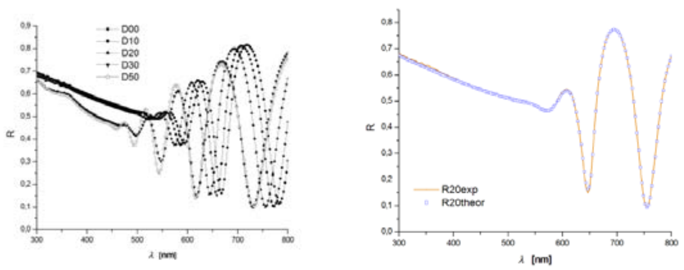

Fig.1: a) *Spectral reflectance of aSi:H/glass thin films prepared under various hydrogen dilution D conditions by the PECVD technique,* b) *Optimized theoretical reflectance model R20theor (squares) compared with experimental data R20exp (line) for D=20.*

Spectral reflectance of the reference sample SiO_2 on Si substrate with thickness t_{ref} = 952.5 nm is in Fig.2a. Positions of the interference fringes were dermined by numerical derivation dR/dλ and used for determination of the film thickness according to Eq.(5-6). Resulting value t_{model} = 952.4 nm is in good agreement with the reference value t_{ref}. PSD plot indicating thickness of the TiO_2/glass film is in Fig.2b. We observe the peak position in the PSD plot exactly in the position corresponding the TiO_2 film thickness.

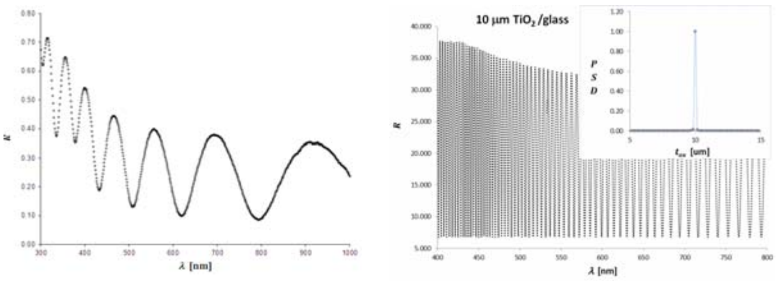

Fig.2: a) *Spectral reflectance of thermal SiO_2/Si, reference film thickness t = 952.5 nm,* b) *Spectral reflectance of 10μm TiO_2/glass sample R(TiO_2) and PSD(R(TiO_2)) plot.*

Ellipsometric spectrum of the SiO_2/Si sample is shown in Fig.3. Thickness of the oxide layer determined from constructed theoretical model is t = 348.78 nm.

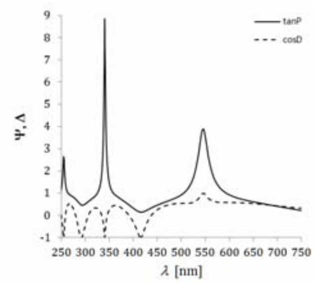

Fig.3: a) *Ellipsometric spectrum Ψ and Δ from the SiO_2/Si experiment.*

Thickness of the SiO_2 layer t = 348.81 nm determined by using Eq.(9) is in good agreement with the previous result.

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