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LETTER TO THE EDITOR

ERRORS ARISING FROM SURFACE ROUGHNESS IN ELLIPSOMETRIC MEASUREMENTS

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A problem of importance to many investigators is the effect of surface imperfections on the measured thickness and refractive index of a thin film overlaying that surface. In this paper, errors produced by neglecting the roughness of the surface are presented. The dimensions of the roughness (submicroscopic bumps and pits) are assumed much smaller than the wavelength of visible light. In this case, the roughness is equivalent on optical properties to a thin flat film on a flat substrate surface. Generally this film is inhomogeneous and anisotropic (uniaxial with its optic axis normal to the surface). The thickness of the equavalent film is arbitrarily made equal to the volume per unit area of all bumps or pits. The principal values of refractive index, or components of polarizability tensor of this equivalent film are determined by the shape of the bumps or pits and surface irregularities associated with them, and by refractive index of substrate. To determine the magnitude of the errors arising from surface roughness in ellipsometric measurements, values of ellipsometric angles Δ and ψ were calculated by representing the rough surface as an equivalent film placed upon a smooth substrate. Two different models were used for this film.

In the first model the equivalent film was considered as inhomogeneous film. A procedure for treating an inhomogeneous (equivalent) film normal to a surface as a series of homogeneous films has been reported previously[1]. The factor $q(z)$ for the random rough surface described by random function of position $z(xy)$ was derived in the form[2]

$$q(z) = \frac{1}{2}\left[1 \mp \Phi\left(\frac{z}{\sigma}\right)\right], \tag{1}$$

where $q(z)$ is the volume fraction of the substrate material in a rough surface versus distance from the mean level and σ standard deviation (— assuming that the random variable z is a normal process with mean zero and standard deviation σ),

$$\Phi = \frac{2}{\sqrt{2\pi}} \int_{0}^{\frac{z}{\sigma}} \exp\left(-\frac{t^2}{2}\right) \mathrm{d}t.$$

Substituting (1) into Maxwell-Garnett relationship[3,4] are calculated of the effective complex refractive index of the equivalent film and using a numerical procedure described in Ref.[1] are calculated ellipsometric angles Δ and ψ. The values of Δ and ψ obtained are given in Figs. 1, 2 for two substrate (silicon and germanium) materials. The analytic solutions are represented by solid lines in Figs. 1, 2, the

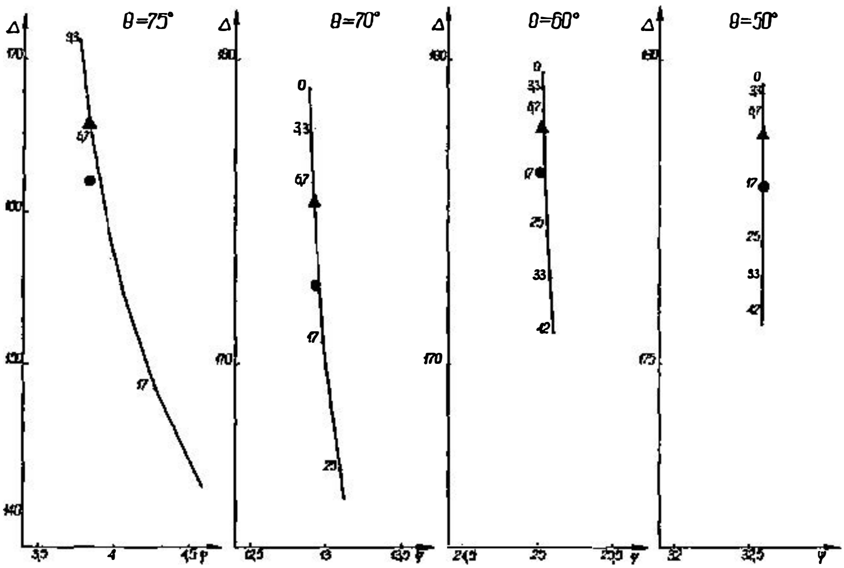

Fig. 1. The solid lines curves were calculated from Maxwell-Garnett relationship, for the factor $q(z)$ in the form (1) and for the angles of incidence 50°, 60°, 70°, 75°, The experimental measurements are presented for silicon by middle points of the series of samples, one in which the surface roughness is small $\delta \le 100$ A° and the other in which the samples have large values of roughness

$$100\ \mathrm{A^\circ} \le \delta \le 200\ \mathrm{A^\circ}$$

These points are presented by the symbols

▲ $0 \le \delta \le 100$ A°

● 100 A° $\le \delta \le 200$ A°

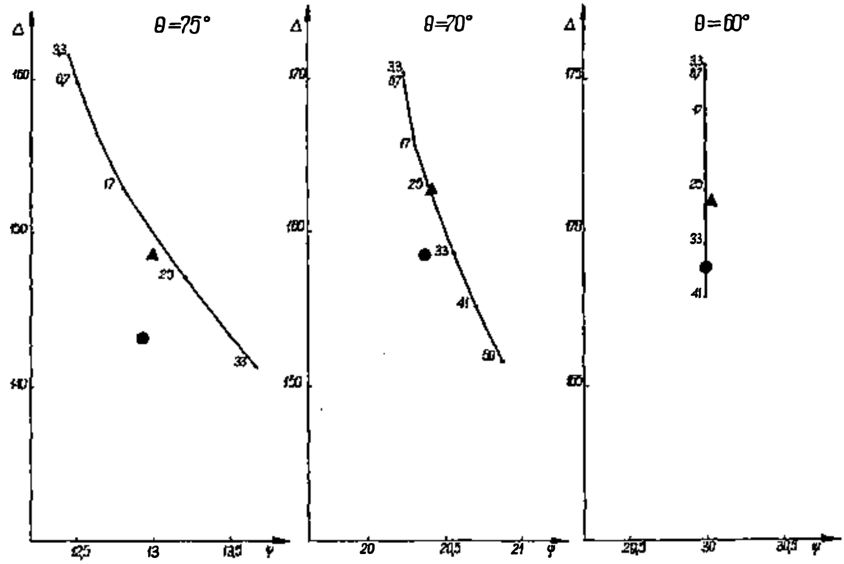

Fig. 2. The solid line curves were calculated from Maxwell-Garnett relationship, for the factor $q(z)$ in the form (1) and for the angles of incidence 60°, 70°, 75°. The experimentatl measurements are presented for germanium by middle points of the two series of samples, one in which the surface roughness is small $\delta \leq 100$ A° and the other in which the samples have larger values of roughness

$$100 \text{ A}^\circ \leq \delta \leq 200 \text{ A}^\circ.$$

These points are presented by symbols

▲ $0 \leq \delta \leq 100$ A°,

● 100 A° $\leq \delta \leq 200$ A°.

experimental results by middle points of the two series of measurements. In the first series the surface roughness of samples is small ($\sigma \lesssim 100$ A°) in the other one is larger ($\sigma \lesssim 200$ A°). The fit of analytic curves to the experimental points in Figs. 1 and 2 for large angles of incidence is not good. With the second model, the problem of the perturbation of reflectance by random distribution of particles on flat substrate surface is considered. Similar problem was previously solved in other ways in Refs.[5-7]. The size of these particles is small compared with the wavelength of incident radiation. Particles are assumed resting on flat substrate surface. In this case the surrounding field is distorted by its image in the substrate. For that reason can be assumed as the first-order approximation for the polarizability tensor of particles expressions

$$\begin{aligned} a_{xx} &= \overset{\circ}{a}_{xx} \frac{2}{1+n^2}, \\ a_{yy} &= \overset{\circ}{a}_{yy} \frac{2}{1+n^2}, \\ a_{zz} &= \overset{\circ}{a}_{zz} \frac{2n^2}{1+n^2}, \end{aligned} \qquad (2)$$

where $\alpha^{\circ}_{xx, yy, zz}$ are diagonal component of the polarizability tensor of an isolated particle and n refractive index of the substrate material. The thin layer of oscillating dipoles (particles) on the surface of a semi-infinite isotropic substrate will contribute an amplitude reflected beam for the cases of „s„ and „p„ polarization separately. It can be shown easily[2] that the total amplitude reflectance are, to first order in perturbation

$$R_s = \left[1 + i\frac{2\pi t}{\lambda} \cdot \frac{4\pi X_{xx}}{\sqrt{n^2 - \sin^2\Theta} - \cos\Theta}\right] \cdot R_{0s}$$

$$R_p = \left\{1 + i\frac{2\pi t}{\lambda}\left[4\pi X_{yy}\frac{\cos\Theta\sqrt{n^2 - \sin^2\Theta}}{n^2\cos\Theta - \sqrt{n^2 - \sin^2\Theta}} + \right.\right.$$

$$\left.\left. + - 4\pi X_{zz} \cdot \frac{n^2 \sin^2\Theta}{n^2\cos\Theta - \sqrt{n^2 - \sin^2\Theta}}\right]\right\} \cdot R_{0p}, \tag{3}$$

where $X_{xx, yy, zz}$ are diagonal component of the electric susceptibility tensor, t thickness of the equivalent film, n refractive index of the material of substrate and of particles, R_{0p}, R_{0s} the Fresnel coefficient for the „p„ and „s„components of amplitude reflected by perfectly smooth surface, Greek Θ the angle of incidence, and Greek λ the wavelength in vacuum. From (3) can be found the ratio of amplitudes

$$\frac{R_p}{R_s} = \operatorname{tg}\psi e^{i\Delta} = \operatorname{tg}(\psi_0 + d\psi)\, e^{i(\Delta_0 + d\Delta)}, \tag{4}$$

and the expressions for the perturbation of the ellipsometric angles

$$d\Delta = \frac{2\pi t}{\lambda}\operatorname{Re}(Z)$$

$$d\psi = -\frac{2\pi t}{\lambda}\sin\psi_0\cos\psi_0\operatorname{Im}(Z), \tag{5}$$

where

$$\operatorname{tg}\psi_0\, e^{i\Delta_0} = \frac{R_{0p}}{R_{0s}}$$

$$Z = 4\pi X_{yy}\frac{N\cos\Theta}{n^2\cos\Theta - N} - 4\pi X_{xx}\frac{1}{N - \cos\Theta} - 4\pi X_{zz}\frac{n^2\sin^2\Theta}{n^2\cos\Theta - N},$$

$$N = \sqrt{n^2 - \sin^2\Theta}. \tag{6}$$

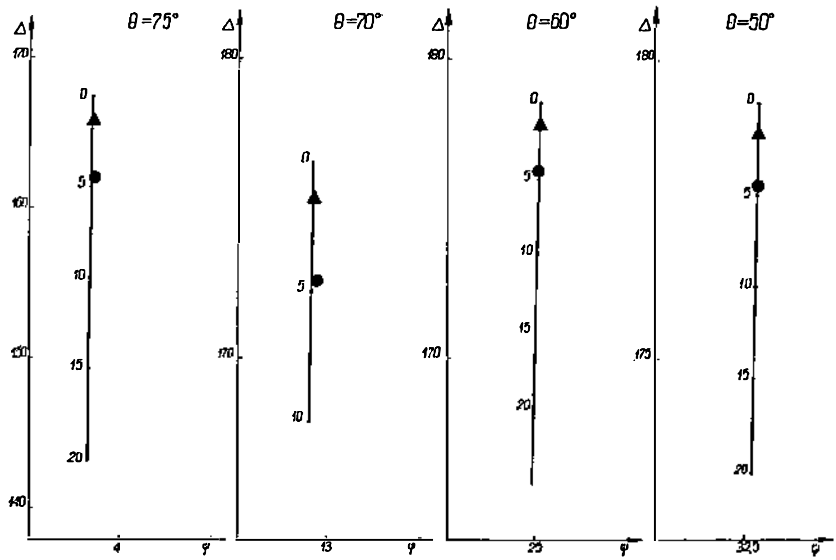

Fig. 3. The analytic solutions for the second model are presented by solid lines curves for the angles of incidence 50°, 60°, 70°, 75°. The experimental points (middle points) for silicon are presented by symbols

▲ $0 \leq \delta \leq 100$ A°

● $100 \leq \delta \leq 200$ A°.

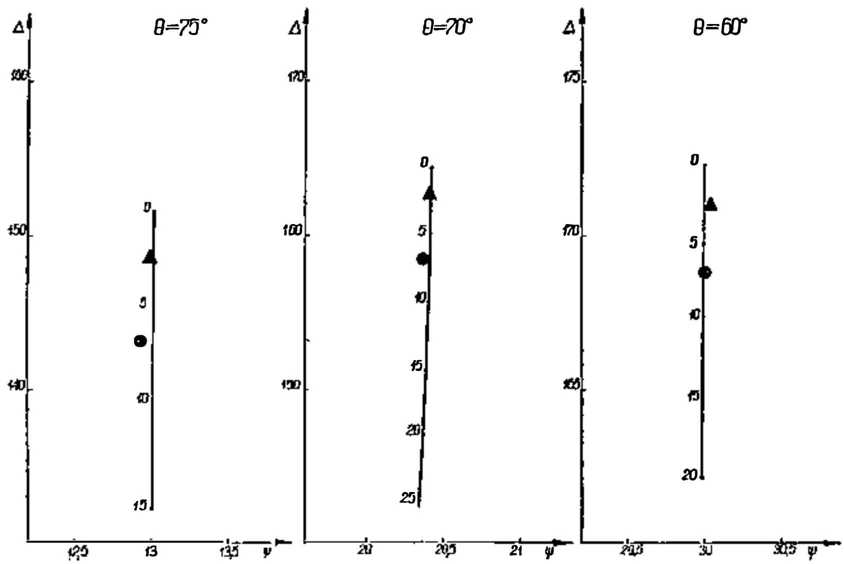

Fig. 4. The analytic solutions for the second model are presented by solid lines curves for the angles of incidence 60°, 70°, 75°. The experimental points (middle points) for germanium are presented by symbols

▲ $0 \leq \delta \leq 100$ A°,

● 100 A° $\leq \delta \leq$ 200 A°.

From (4) and (5) can be obtained (in the first-order approximation in t/λ) expressions for the ellipsometric angles Δ and ψ as functions of surface roughness.

$$\psi(t) = \psi_0 - \frac{2\pi t}{\lambda} \sin\psi_0 \cos\psi_0 \,\mathrm{Im}(z),$$
$$\Delta(t) = \Delta_0 + \frac{2\pi t}{\lambda} \mathrm{Re}(z). \qquad (7)$$

Because for the silicon and germanium refractive index

$$n \gg 1$$

and

$$X_{zz} \gg X_{xx} = X_{yy}$$

Equs. (7) simplify to[2]

$$\Delta(t) = \Delta_0 - \frac{2\pi t}{\lambda} \mathrm{tg}\,\Theta \sin\Theta \,\mathrm{Re}(4\pi X_{zz}),$$
$$\psi(t) = \psi_0 + \frac{2\pi t}{\lambda} \mathrm{tg}\,\Theta \sin\Theta \sin\psi_0 \cos\psi_0 \,\mathrm{Im}(4\pi X_{zz}). \qquad (8)$$

To carry the calculation further, we must assume a particular type of the particles on the surface. The calculations were made for a sparse distribution of spheres. The values of Δ and ψ obtained from the calculations are given in Figs. 3 and 4. The analytic solutions are represented by solid lines, the experimental results by middle points of two series of measurements (analogous to Figs. 1 and 2). Figs. 3 and 4 show a good fit of the analytic curves to the experimental points.

From the previous Refs. [1,2,4,7] and our results the following conclusions can be drawn:

- the dependence of the measured ellipsometric angles Δ and ψ on surface roughness for silicon and germanium was observed,
- a good agreement between the analytic curves and the experimetal data was obtained for the second model, and
- errors produced by neglecting the roughness of the surface can be relatively large for silicon and germanium.

Our results[2] obtained from ellipsometric measurements in the region surface roughness

$$0 \leq \sigma \leq 200\ \mathrm{A}^\circ$$

confirm these conclusions.

References

1) C. A. Fenstermaker and F. L. McCrackin, Surf. Sci., **16** (1969) 85;

2) K. Brudzewski, Dissertationt Technical University of Warsaw, 1973;

3) M. Garnet, Phil. Trans. Roy. Soc. London **203** (1904) 384; **205**, (1906) 237;

4) O. S. Heavens, Optical Properities of Thin Solid Films, (Butterworths, London, (1955), Ch. **6** p. 177.

5) C. S. Strachan, Proc. Cambridge Phil. Soc. **29** (1933) 116;

6) D. W. Berreman, Phys. Rev. **1**, **B2** (1970) 381;

7) D. W. Berreman, JOSA, **60**, **4** (1970) 499.