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Ellipsometric Studies of SiO_2 Films on Si Substrates

Badania elipsometryczne warstw SiO_2 na podkładkach Si

Эллипсометрические исследования пленок SiO_2 на подложках Si

1. INTRODUCTION

Ellipsometry is an optical technique for the determination of the optical constants of surfaces and layers by the measurement of the changes in the state of polarization of light upon reflection from the measured materials. The reviews of research on this subject were given by Azzam and Bashara [1] and by Rzhanov [2] .

We present an example of the application of the method of ellipsometry for characterization of SiO_2 passive layers on

Si nuclear detectors. The layers have been produced by anodic oxidation and a solution of KNO_3 in ethyleneglycol served as an electrolyte. The details of the samples preparation will be given in another paper.

2. DESCRIPTION OF THE EQUIPMENT SET-UP

A basic schematic diagram of the optical system is shown in Fig. 1. We use a light beam from argon ion ILA 120 or He-Ne

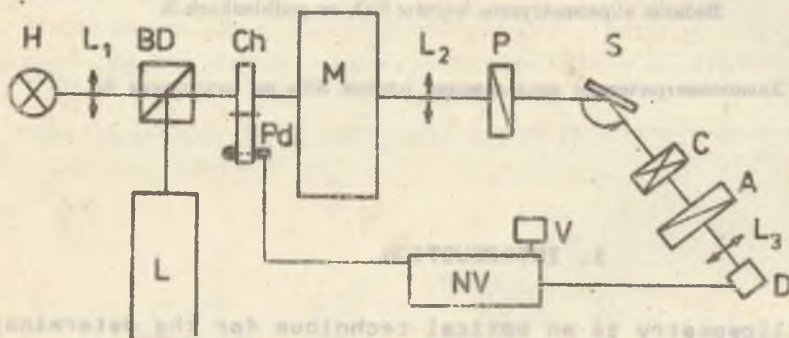


Fig. 1. Schematic diagram of the ellipsometer: H - halogen lamp, $L_{1,2,3}$ - lens, BD - beam divider, Ch - chopper, Pd - photodiode, M - monochromator, P - Glan-Thompson polarizer, S - sample, C - Soleil-Babinet compensator, A - Glan-Thompson analyser, D - detector, NV - lock-in nanovoltmeter, V - digital voltmeter, L - laser

laser, or light from the 250 W halogen lamp that was focused by lens on the entrance slit of a wide-wavelength range monochromator SPM-2 Zeiss. The emergent light is collimated by the second lens and passes through an ellipsometer of our construction.

The instrument has two arms, the first with a Glan-Thompson polarizer is situated on the optical axis of the monochromator. The second, moving arm is composed of a sample mount with a goniometer, a Soleil-Babinet compensator, a Glan-Thompson analyzer and a photodetector. A special construction of a gearing mechanism allows a sample table to rotate through half the angle of a moving arm. This makes possible to set any desired angle in the interval from 14 to 180 degrees, up to the angle of incidence of 87°. The light from the laser passes through monochromator to cut off the plasma emission. The apparatus shown in Fig. 1. works in a PSCA /Polarizer, Sample, Compensator, Analyser/ arrangement, It can also be changed to a PCSA sequence.

Different photodetectors /photomultipliers, silicon phototransistors or PbS resistors/ can be used, depending on the wavelength. Soleil-Babinet compensator with a retardation phase set equal to 90° is mounted in the centre of a rotatable table. The accuracy of reading of the azimuthal angles of the compensator and of the polarizers is better than 1 minute.

The ellipsometer has been calibrated with a standard glass plate of a given refraction index and with an evaporated gold layer.

3. MEASUREMENTS AND CALCULATIONS

Our ellipsometer worked with a He-Ne laser /6328 Å /, a suitable light source for a SiO₂/ Si system, and with the angle of incidence of 70°. This instrument is "null's" type. The null ellipsometry is based on finding a set of azimuthal angles for the polarizer, compensator and analyzer / γ_P , γ_C , γ_A /, such that the light flux falling on the photodetector is extinguished.

The ellipsometric parameters, the change in phases Δ and in amplitudes Ψ of parallel /p/ and perpendicular /s/ components of linearly polarized light when it is reflected from the surface, can be determined using equations [2] :

$$\Delta = -2\gamma_A + 2\gamma_C + \nu + 2m\pi \quad /1/$$

$$\operatorname{tg} \Psi = \operatorname{tg} \gamma_P \sqrt{\frac{1 - \cos 2\gamma_C \cos (2\gamma_A - 2\gamma_C)}{1 + \cos 2\gamma_C \cos (2\gamma_A - 2\gamma_C)}} \quad /2/$$

where
$$\operatorname{tg} \nu = \frac{(\sin 2\gamma_C - 1) \cdot \operatorname{tg} (2\gamma_P - 2\gamma_C)}{\sin 2\gamma_C + \operatorname{tg}^2 (2\gamma_P - 2\gamma_C)}$$

Suppose that the SiO_2 films on Si substrate are all optically isotropic and homogeneous, with plane homogeneous boundaries. The fundamental equation of ellipsometry for this system is [1] :

$$\operatorname{tg} \Psi e^{i\Delta} = \frac{(r_{1p} + r_{2p} e^{-2i\delta})}{(1 + r_{1p} r_{2p} e^{-2i\delta})} \cdot \frac{(1 + r_{1s} r_{2s} e^{-2i\delta})}{(r_{1s} + r_{2s} e^{-2i\delta})} \quad /3/$$

where r_{1p} , r_{2p} , r_{1s} , r_{2s} are Fresnel reflection coefficients for two interfaces: ambient-film and film-Substrate:

$$r_{1p} = \frac{N_1 \cos \phi_0 - N_0 \cos \phi_1}{N_1 \cos \phi_0 + N_0 \cos \phi_1}$$

$$r_{2p} = \frac{N_2 \cos \phi_1 - N_1 \cos \phi_2}{N_2 \cos \phi_1 + N_1 \cos \phi_2}$$

$$r_{1s} = \frac{N_0 \cos \phi_0 - N_1 \cos \phi_1}{N_0 \cos \phi_0 + N_1 \cos \phi_1}$$

$$r_{2s} = \frac{N_1 \cos \phi_1 - N_2 \cos \phi_2}{N_1 \cos \phi_1 + N_2 \cos \phi_2}$$

N_0, N_1, N_2 are complex refractive indices of ambient /air/, film and substrate, respectively. The angles of incidence ϕ_0, ϕ_1, ϕ_2 in 3 media are interrelated by Snell's law:

$$N_0 \sin \phi_0 = N_1 \sin \phi_1 = N_2 \sin \phi_2$$

$$N = n - ik$$

δ is a phase change caused by the presence of a film of thickness d and index of refraction n_1 :

$$\delta = \frac{2\pi}{\lambda} d [n_1^2 - \sin^2 \phi_0]^{1/2}$$

Two parameters of a substrate: n_2 and extinction coefficient k_2 can be calculated from Δ and ψ measured on the unoxidized parts of the samples, using equations [3]:

$$n_2^2 - k_2^2 = \sin^2 \phi_0 / 1 + \operatorname{tg}^2 \phi_0 \frac{\cos^2 2\psi - \sin^2 2\psi \sin^2 \Delta}{1 + \sin^2 \psi \cos^2 \Delta / 2} / 4$$

$$2n_2 k_2 = \sin^2 \phi_0 \operatorname{tg}^2 \phi_0 \frac{\sin 4\psi \sin \Delta}{1 + \sin^2 \psi \cos^2 \Delta / 2}$$

Using the ellipsometer of our construction we performed measurements of HF-etched Si substrates and Si covered with the anodic oxide layers. For different samples the conditions of the oxidation were the same.

The obtained values of refractive index and extinction coefficient of crystalline Si substrates /Tab. 1/ are in good agreement with literature values, which are well established now [4]. The fundamental absorption edge of the silicon oxide lies in the ultraviolet region and at 6328 Å the films are

transparent ($k = 0$). Two parameters of our samples: n_1 and the thickness of the film d are still unknown. They can be determined by a numerical search through various values of n_1 and d , that satisfy eq./3/ with values of ψ and Δ taken from the measurement. The results for six Si detectors with different passive oxide layers are given in Tab. 1.

Tab. 1. Optical constants and oxide thicknesses of Si nuclear detectors

Sample	n_1	d/nm	n_2	k_2
1	1.621	92,2	3.862	0,021
2	1.619	87,6	3.860	0,022
3	1.624	74,1	3.873	0,020
4	1.628	76,0	3.875	0,021
5	1.619	79,3	3.902	0,023
6	1.611	66,3	3.897	0,022

4. CONCLUSIONS

We have shown that instrument described in this paper can be used as a sensitive tool for measuring the optical properties of the oxide/substrate structures and determining the oxide layer thicknesses. The value of refractive index gives information on quality and composition of produced anodic oxidized films. In our case these values are large compared with values for SiO_2 taken from the literature [5, 6], which lie in the range $1.45 + 1.50$. For SiO the refractive index approaches value of 2 at 6328 \AA [6]. Mostly probably the admixture of silicon monoxide phase in our films exists. More detailed studies connected with the influence of a method of oxide layer preparation on optical properties of the structures will be performed.

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STRESZCZENIE

W pracy opisano budowę elipsometru do pomiarów spektroskopowych, pracującego wraz z monochromatorem SPM-2. Wyznaczono stałe optyczne i grubości warstw tlenkowych detektorów jądrowych wykonanych z krzemu.

Р Е З Ю М Е

В работе представлен эллипсометер позволяющий производить спектроскопические исследования с монохроматором СПМ-2. Определено оптические постоянные и толщины окисных пленок на кремниевых подложках ядерных детекторов.

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