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Determination of optical parameters of CdTe films by principal angle ellypsometry

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The principal angle and ellipticity of the light wave reflected from the surface of the single-crystal silicon coated by a CdTe film have been measured in 366–579 nm spectral region. Using a specially developed computer graphic program of the ellipsometric data processing optical constants and a film thickness distribution over the sample surface area have been determined. The CdTe refraction index values obtained for the film are considerably lower than that of CdTe single crystal. That is explained by porous structure of the film.

В спектральной области 366–579 нм измерены главный угол и эллиптичность световой волны, отраженной от поверхности монокристалического кремния, покрытой пленкой теллурида кадмия. Представлена компьютерная графическая программа обработки эллипсометрических измерений, с помощью которой найдены оптические постоянные и распределение толщины пленки по площади образца. Полученные значения показателя преломления пленки теллурида кадмия значительно меньше показателя преломления монокристалического CdTe, что объясняется рыхлой структурой пленки.

Semiconductor films are widely used in development of solar energy converters and signal transmission devices. In particular, CdTe thin films are used in electroluminescence devices as emitters as well as for protection of light energy receiver surfaces in near infrared spectral region. To design the film devices, it is necessary to know optical parameters of film and its thickness, distributing of the film thickness over the surface area, the radiation and chemical resistance of film structures. The reflective ellipsometry based on the analysis of polarization characteristics of the wave reflected from the tested sample is an effective film control method. In this work, a computer program for graphic processing of the ellipsometrical data obtained by principal angle ellipsometry and determination of optical parameters (refraction and absorption indices) and thickness of a film. The program is checked taking as an example a CdTe semiconductor film deposited onto silicon single crystal. It is to note that optical properties of CdTe films on silicon are scarcely studies up to now. The known data [1–4] on CdTe films on other substrates show that the surface structure and optical parameters of the film depend considerably on the deposition conditions. Therefore, the technology of film structures requires convenient and reliable non-contact control methods.

Studied was a thin CdTe film obtained by the vacuum epitaxial "hot wall" method. The film preparing technology has been described in details elsewhere [6]. The sample was shaped as a thin (~1 mm) plate of single-crystalline Si coated in its central part with the film spot of about 20 mm diameter. The coating thickness within limits of the spot was varied along the radial direction, what the corresponding distribution of the interference coloring testified about. The ellipsometric measurements were carried out at 579, 546, 435, 405 and 366 nm wavelengths of a mercury lamp emission spectrum using a home-made photometric ellipsometer with variable incidence angle,

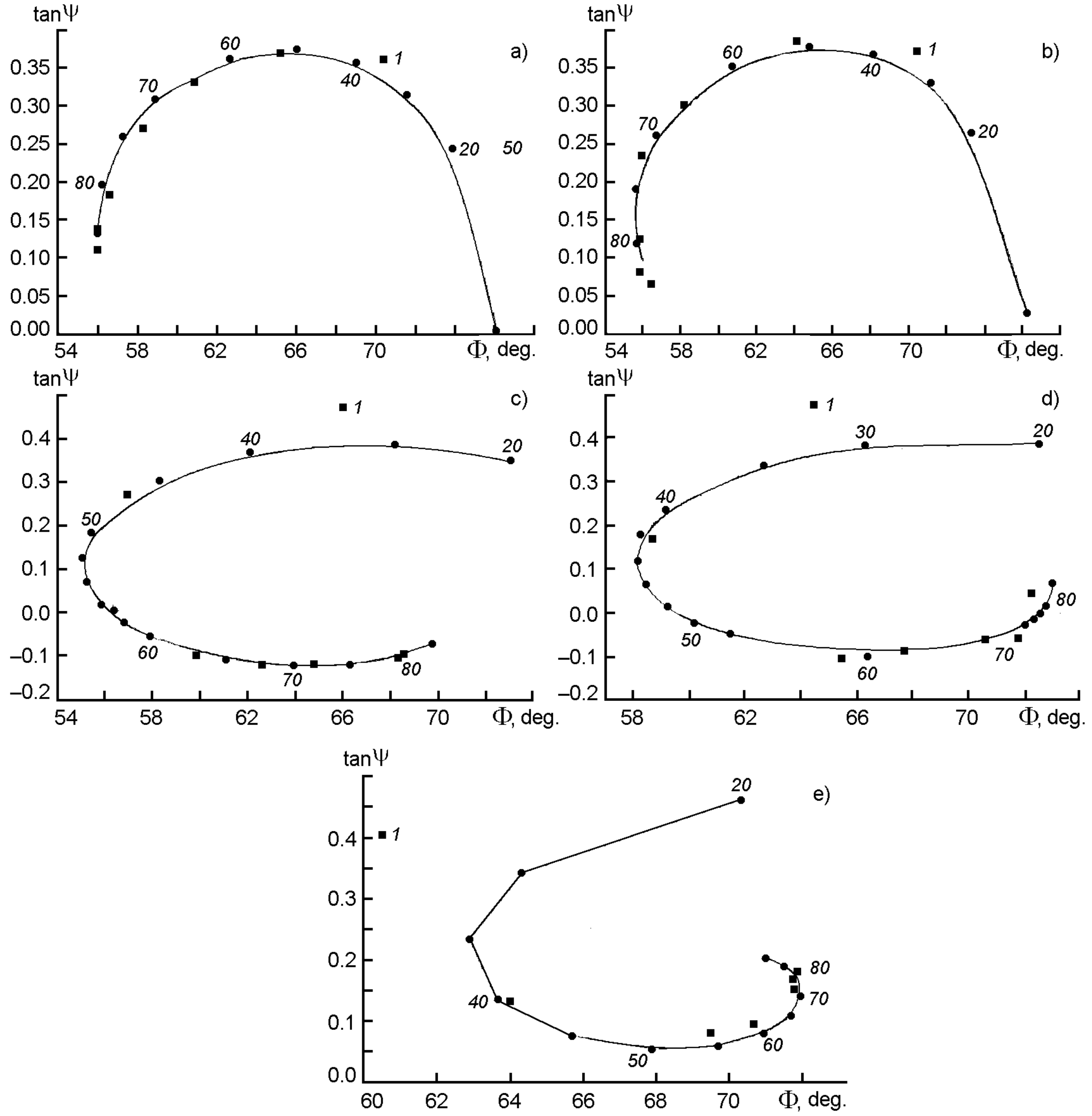

Fig. 1. Ellipsometric parameters Φ and tgψ (points) measured on several wavelengths (a–e) at light reflection from different sample areas in comparison with the values calculated using the ellipsometry equation in the single-layer model of the reflective system (continuous curves). The numbers near marks on theoretical curves indicate the layer used in of calculations are presented in the Table.

calibrated using a single-crystal silicon plate. The ellipsometer has been designed according to the non-compensated "analyzer-sample-polarizer" scheme. In the used modification of photo-electric ellipsometric method [7], the ellipsometric parameters cosΔ and tgΨ are the measured values, where Δ is the phase difference between the p- and s-component of the reflected light wave electric vector, and tgψ, the ratio of reflection coefficient in the incidence plane (p-plane) to that in the s-plane perpendicular thereto. The ellipsometrical parameters are determined by measuring intensities I_0, I_{45}, I_{90}, I_{-45} of radiation reflected from the sample at four azimuths of the analyzer according to 0°, 45°, 90°, −45° respectively with respect to the incidence plane and at a fixed azimuth of polarizer ψ_Π:

$$\mathrm{tg}\psi = \mathrm{tg}\psi_\Pi \sqrt{\frac{I_0}{I_{90}}},$$

$$\cos\Delta_1 = \frac{2I_{45} - I_0 - I_{90}}{2\sqrt{I_0 I_{90}}},$$

$$\cos\Delta_2 = \frac{I_{45} - I_{-45}}{2\sqrt{I_0 I_{90}}}.$$

Table. Optical constants n_2 and κ_2 and thickness of investigated film

λ, nm	Si [8, 9]		Film		Film on an area 1		Region of thikness film (nm)		CdTe [12, 13]	
	n_3	κ_3	n_2	κ_2	n_2	κ_2	d_{2min}	d_{2max}	n_2	κ_2
579.06	4.04	0.030	2.08	0.40	1.90	0.20	34	85	3.02	0.38
546.07	4.08	0.042	2.10	0.38	1.70	0.20	33	83	3.06	0.42
435.83	4.56	0.185	2.35	0.34	2.10	0.34	39	84	3.27	0.69
404.65	5.43	0.350	2.55	0.41	2.10	0.40	36	75	3.39	0.90
366.00	6.52	2.705	2.60	0.80	2.15	0.75	38	80	2.90	1.53

The phase difference Δ is found as average of Δ_1 and Δ_2. Before measuring, the ellipsometer should be adjusted according to [7].

It is well known that the sensitivity of ellipsometric parameters to characteristics of the reflecting system is the highest if the measurements are carried out at the so-called principal angle, i.e., angle of incidence φ at which $\Delta = 90^\circ$ ($\cos\Delta = 0$). In this work, the principal angle and tgψ at this angle (ellipticity) have been found by measuring the ellipsometricl parameters at three angles of incidence on both sides from the principal one but near thereto, that is, at those angles where $\cos\Delta$ changes its sign and its values are within limits $\cos\Delta \approx \pm 0.1$. Really, the angle of incidence was to be varied within ±15 angular minutes with respect to the principal angle. In most cases of non-thick films, $\cos\Delta$ in the such small angular interval varies linearly and tgψ remains essentially unchanged, therefore, the principal angle value was found by linear interpolation of $\cos\Delta = f(\psi)$ dependence. The probing light beam was directed to areas with a different interference coloring (up to seven areas) located along the spraying spot radius, that allowed to determine the distribution of the film thickness and optical constants over the sample surface area.

Let the measurement results be presented as diagrams where the measured values of ellipsometric parameters, principal angle Φ and ellipticity tgψ, are laid on orthogonal axes, then every pair of these values will be represented by a point on the diagram.

Fig. 1 presents the experimental data obtained at the light reflection from different areas of the sample. The experimental points on the diagram are seen to form sections of a spiral. This is seen especially well for short wavelengths. As these points are obtained at the light reflection from areas of different thickness, it is believed that the curves correspond to permanent values of optical constants, along each curves the layer thickness varies while its optical constants remain unchanged. Natural is to assume also that the investigated layers are absorbing, since the intrinsic absorption region of the layer material (cadmium telluride) lies just in the visible part of spectrum. The optical constants of substrate (single-crystalline silicon) are well known [2, 3], thus, it is the film optical constants n_2, κ_2 and its thickness d_2 are to be determined.

The fitting procedure of refraction (n_2) and absorption (κ_2) indices of CdTe films was carried out using a special graphic program. All calculations were made using a of software package [4, 5]. The fitting results of theory to experimental data are presented in Fig. 1 as the corresponding curves. In the Table, the substrate parameters (single-crystalline Si) used in computations are given as well as the obtained values of the CdTe film thickness and optical constants in comparison with optical constants of CdTe single crystal.

It is seen from results presented in Fig. 1 that theoretical curves describe well the experimental results, passing the experimental points for most areas. However, the point for the area 1 (where, judging from the interference coloring, the film thickness is the smallest) for all wavelengths of the studied range does not get on theoretical curves disposed in that region of diagram where the refraction indexes are considerably lower than those for theoretical curves. Judging from the experimental point location, we estimate the film thickness in this area as $d_2 = 30$–40 nm. The film optical constants for that area are calculated by an iterative method [4], the layer thickness in the being assumed to be of 35 nm. The film optical constants for that area are shown in separate columns of the Table.

It is evident from the data presented in the Table that the film thickness range found from measuring on different wavelengths is essentially the same. This can testify to reliability of the method used to calculate the film parameters. The thickness values for corresponding areas obtained from ellipsometric data for different wavelengths coincide to within $\Delta d_2 = \pm 2$ nm; that value can be acceptes as the error of the applied film thickness determination procedure. In the studied spectral region, the refraction index increases as the wavelength diminishes, and its values are substantially lower than that of single-crystalline CdTe, unlike the absorption index which is only a bit lower than that of CdTe.

In our opinion, this is caused by the fact that the studied film is not single-crystalline but is loose, having a changed structure which includes pores between the separate grains of basic material. In accordance with data of X-ray diffraction [6], the film structure is polycrystalline. The pores in the film bulk contain air, thus, the effective refraction index of the film is lower than that of continuous material. Obviously, the porosity degree decreases as the film thickness increases, so the refraction index grows. Such structure of films is expectable; since the lattice constants of silicon (5.4282 Å) and CdTe (6.477 Å) differ considerably, formation of epitaxial single-crystalline structures for that pair of materials is hindered.

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Визначення оптичних параметрів плівки телуриду кадмію методом еліпсометрії головного кута

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В спектральній області 366–579 нм виміряно головний кут і еліптичність світлової хвилі, відбитої від поверхні монокристалічного кремнію, вкритою плівкою телуриду кадмію. Представлено комп'ютерну графічну програму обробки еліпсометричних вимірів, з допомогою якої знайдено оптичні сталі та розподіл товщини плівки по площі зразка. Одержані значення показника заломлення плівки телуриду кадмію значно менші за показники заломлення монокристалічного CdTe, що пояснюється пухкою структурою плівки.