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Optical Properties of CdS/CdTe Heterojunction Prepared by Physical Vapor Deposition Technique

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The paper presents the study of the optical properties of a thin layer of Cadmium Sulphide deposited on Cadmium Telluride films. CdTe thin films were obtained by vapor phase condensation method using different technological factors, in particular, different thickness (different time of deposition τ) on glass substrates. After deposition the optical properties were analysed by Swanepoel method, using transmission spectra. The upper thin layer of CdS was deposited by thermal evaporation method on CdTe thin films. The change in optical properties of CdS/CdTe heterojunction in comparison with CdTe thin films was investigated. Using a Swanepoel method were calculated the main optical constants, such as refractive index, absorption coefficient and optical conductivity. By this method the thickness of the thin film was determined and compared with the experimental values obtained by the profilometer.

Keywords: thin films heterojunction, thermal evaporation method, optical properties.

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Introduction

Thin film PV solar cell has been considered one of the promising solar cells due to its high energy conversion efficiency, low cost and convenience for large scale production. The most successful thin film solar cells have been cadmium telluride (CdTe), copper indium gallium selenide (CIGS) and amorphous silicon (a-Si) with efficiencies of 18.3 %, 20 % and 12.3, respectively [1]. Typically, the efficiencies of thin-film solar cells are lower compared with silicon (wafer-based) solar cells, but manufacturing costs are also lower. It was reported that [2], CdTe technology costs about 30% less than CIGS technology and 40% less than A-Si technology.

The theoretical efficiency of CdS/CdTe solar cells is predicted to be up to 28 – 30 % [3, 4]. However, the real efficiency of PV solar cells based on the n-CdS / p-CdTe heterojunction in a superstrate structure is currently 20.4 % [5], and the efficiency of solar modules with an area > 1 cm^2 is 16.5 % [6, 7] The major impact factors for this difference are due to the optical losses, surface recombination, recombination in the space-charge region and rear contact effect.

The best small-area CdTe thin-film cells manufactured show more than 15 % conversion efficiency [8]. Large-area modules with aperture efficiencies in excess of 10 % have also been demonstrated (Ullal et al., 2000). First Solar (the largest CdTe manufacturer) reported fleet average efficiencies increasing from 12.9 % in 2012 to 16.6 % in 2016 for their CdTe modules (First Solar, 2017). For CdTe cells, module efficiency record for the moment is 18.6 %. The best CIGS reported efficiencies so far were 17.5 % for modules (Green et al., 2017). There is also significant industrial production based on CdTe/CdS solutions, represented to a large extent by American corporation First Solar, which is a supplier of PV modules used in the currently largest Agua Caliente Solar Project solar power plant in Arizona [9]. It should be noted that thin film technology based on CdTe is the first technology that has allowed to low the production costs of solar energy up to 0.57 $/W [10]. In spite of the 10 % difference in the lattice constants of CdS and CdTe, they form an electrically excellent heterojunction, as shown by its high fill factors up to FF = 0.75 in the devices made.

Thin film flexible solar cells using CdS/CdTe semiconductor compounds are currently in active research and in the field of interest of several research centers in the world. This is due to the fact that flexible PV cells have a record high power per unit weight - more than 2 kW/kg [11]. Such characteristics are achieved thanks the construction of a flexible SC, where the glass substrate is replaced by a polyamide film. In recent years there have also been reports of the first attempts to manufacture this type of structures on elastic substrates, including both configurations: superstrate [12-13] and substrate [14].

At present, a lot of methods have been developed for the production of thin CdTe films. This paper presents the thermal evaporation method [15]. In order to calculate the refractive index from optical transmittance data the interference patterns in the transmittance spectra should be suppressed by generating the envelope around transmittance maxima and minima [16]. Than the interference pattern free transmittance spectra of deposited films should be used to calculate the refractive index using Swanepoel method [17].

This straightforward method proposed by Swanepoel [18], based on the use of the extremes of the interference fringes of transmission spectrum only, will be used in order to derive the real and imaginary parts of the complex index and also the thickness for the semiconductor film. Through the use of materials with a higher optical absorption coefficient, it is possible to reduce the thickness of active photovoltaic cell layers [19], which affects not only the decrease in production costs, but also the possible weight reduction of photovoltaic devices depending on the substrate used.

There are number of papers theoretically focused on detailed investigation of the dependence of the efficiency of CdS/CdTe thin film solar cells on some properties [20 - 24]. However, the results of complex experimental studies of the spectral dependences of the main optical constants have been presented a little. Therefore, our studies are of great importance for the further development of highly efficient devices based on heterojunctions for electronics and solar energy.

Experiment Methodology

First the thin films of CdTe were deposited on a cleaned glass substrates by thermal evaporation method. In the used installation can be to receive series (5 - 15 films) in a single cycle for various technological factors: different thickness d = (0.01 - 12) μm at a constant temperature of deposition T_S = (300 - 570) K; uniform thickness *d* with different T_S; different temperature of evaporation T_E (600 - 1070) K with constant thickness *d* or deposition temperature T_S.

Thin films of CdTe for research were obtained with different thicknesses (different deposition time τ) at a constant T_S and T_E (Table 1). The growth temperature T_s was 470 K, the evaporation temperature of pre-synthesized compounds CdTe was T_E = 870 K. The thicknesses of thin films were set by deposition time τ = (60 - 180) sec.

Further the next layer of CdS was deposited on CdTe thin films by thermal evaporation method. The technological parameters shows Table I.

The samples thickness was analysed using profilometer Bruker Dektak XT. Optical transmission spectra was investigated by measuring transmittance, T at normal incidence and room temperature. The measurements were carried out in the wavelength range of 190 – 3300 nm with 1 nm step using Agilent Technologies Cary Series UV-Vis-NIR Spectrophotometer.

Table I

Technological parameters of CdTe and CdS/CdTe thin films

Sample number	Substrate temperature T_S, K	Evaporation temperature T_E, K	Deposition time τ, sec	Thickness d, nm
CdTe/glass				
21	470	820	180	1485
24	470	845	160	1215
CdS/CdTe/glass				
21	470	1150	45	1689
24	470	1150	30	1490

Results and discussion

Optical characterization of thin films gives information about other physical properties, e.g., bandgap energy, band structure, and optically active defects [25]. The effects of thickness and heterojunction properties on the optical transmittance of the CdTe and CdS/CdTe films have been studied. The region of fundamental absorption was observed in transmission spectra. The transmission spectra of CdTe and CdS/CdTe thin films obtained on the glass substrates with different thicknesses were measured in the wavelength range from 180 to 3300 nm and are shown in Figures 1-2. It can be observed that the films are highly transparent in the near infrared region. Absorption edge is about 800 nm for all samples, which is completely consistent with the width of the bandgap of CdTe thin films [26]. In addition, the observed interference patterns in the optical transmission spectra are the indication for the thickness homogeneity of deposited films [27].

On Figs. 1-2 can be seen that for as grown CdTe films the transmission values reach up to 90 %, which also indicates the high transparency of the films. For a thick film CdTe No21 (Fig.1) is observed a smoother growth of the transmittance with a wavelength compared to the sample CdTe No24 (Fig. 2). Here is worth to note, that the number of "interference maxima" also depends on the thickness of the film. This could be explained by the fact that there is a difference between the refractive indexes of the film and substrate and also due to the interference of multiple light reflections Fig. 3 [28].

Transmission values for CdS/CdTe heterojunction are slightly lower than those for pure CdTe films, which may indicate greater reflection or scattering in film thickness.

One of the most popular methods that uses these interference fringes to determine the optical properties of

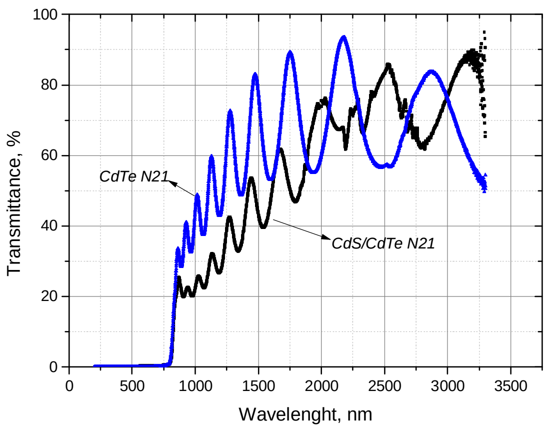

Fig. 1. Optical transmission spectra of CdTe thin film and CdS/CdTe heterojunction (sample 21).

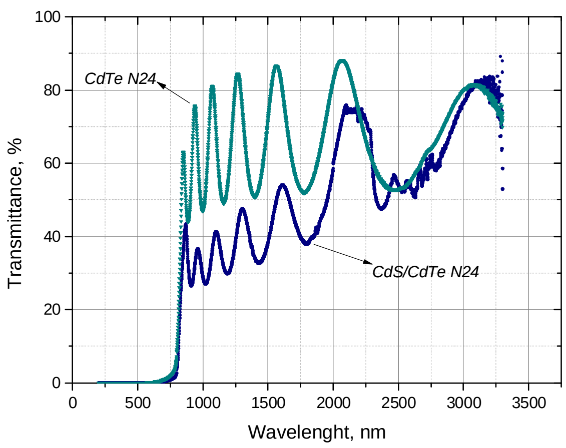

Fig. 2. Optical transmission spectra of CdTe thin film and CdS/CdTe heterojunction (sample 24).

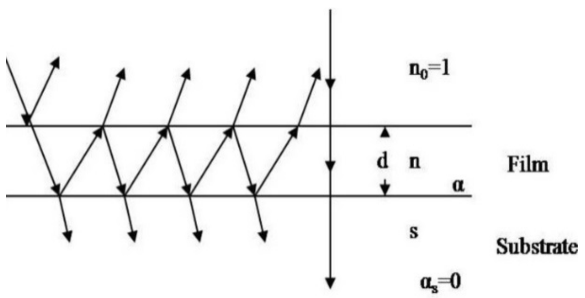

Fig. 3. Schematic diagram of a thin film on the substrate. Arrows indicate transmission and reflection at different interfaces.

the material is the Swanepoel method [29].

The shape of a thin film on a transparent substrate looks like on Fig. 3. In this figure, n, α, d and T denote the refractive index, absorption coefficient, thickness and transmission of the film, respectively. The transparent substrate has a thickness of several orders of magnitude larger with index of refractions and absorption coefficient $\alpha_s = 0$ and transmittance T_s. The index of refraction for air is $n_0 = 1$. If the thickness d is uniform then the interference effects generate a spectrum. The interference fringes can be used to calculate the optical constants of the film such as refractive index, film thickness, absorption coefficient and optical conductivity.

The transmission T for the normal incidence resulted from the interference of the wave transmitted from three interfaces can be calculated as [30]:

$$T = T(n, x) = \frac{Ax}{B - Cx\cos(\varphi) + Dx^2}, \qquad (1)$$

where:

$$A = 16n^2 s \qquad (2)$$

$$B = (n+1)^3(n+s^2) \qquad (3)$$

$$C = 2(n^2-1)(n^2-s^2) \qquad (4)$$

$$D = (n-1)^3(n-s^2) \qquad (5)$$

$$\varphi = \frac{4\pi n d}{\lambda} \qquad (6)$$

$$x = e^{-\alpha d} \qquad (7)$$

Maximum and minimum of interference fringes are determined from the following equations:

$$T_M = \frac{Ax}{B - Cx + Dx^2} \qquad (8)$$

$$T_m = \frac{Ax}{B + Cx + Dx^2} \qquad (9)$$

The refractive index of the substrate is found from the following expression (T_s=max):

$$s = \frac{1}{T_s} + \left(\frac{1}{T_s^2} - 1\right)^{\frac{1}{2}} \qquad (10)$$

From the equations above the refractive index is determined:

$$n = \left(N + (N^2 - s^2)^{1/2}\right)^{1/2}, \qquad (11)$$

where

$$N = \frac{2s(T_M - T_m)}{T_M T_m} + \frac{s^2+1}{2} \qquad (12)$$

Using the equations (11) and (12) and taking into account s = 0.92 the refractive index of samples CdTe and CdS/CdTe can be obtained. The calculated values of refractive index (n) are presented in Tables II-V for CdTe thin films and heterojunction of CdS/CdTe. The refractive index is the range of frequencies in which films are weakly absorbing. Figures 4-5 shows the variation of refractive index of CdTe films and the average value is about 2.48 for a sample No 21 and 2.45 for a sample No 24. This values are completely consistent with the literary ones that matter for CdTe thin films to 2.5 [31]. For heterojunction of CdS/CdTe these values are about 2.52 for a sample No21 and 2.72 for No 24. These values is consistent with literary [32].

The thickness of the film is calculated from the equation:

$$d = \frac{\lambda_1 \lambda_2}{2(\lambda_1 n_2 - \lambda_2 n_1)} \qquad (13)$$

provided that n_1 and n_2 are the refractive indices of the wave's λ_1 and λ_2 calculated for two neighboring maxima or minima. For the samples CdS/CdTe No 21 and CdTe No 21, the thicknesses of the films are presented in Table II and Table III, respectively, as d_1.

Comparing the experimental and calculated values of the thickness, can be note that a small difference in value is associated with the error in experimental studies.

The order of interference m at the maxima of transmission spectra for wavelength λ_1 is:

Table II

Calculated optical properties by Swanepoel method for CdS/CdTe heterojunction (sample 21)

λ, nm	**T_M**	**T_m**	**n**	**d_1, nm**	**m**	**α, cm^{-1}**	**σ_{opt}, 10^{11}**
2000	0.7562	0.5164	2.237				
1790	0.6739	0.4688	2.275				
1672	0.6184	0.4275	2.353	1729.00	3	2700.72	15.0
1543	0.5754	0.3953	2.425	1663.77	4	3069.41	17.5
1443	0.5359	0.3553	2.578	1318.88	4.5	4879.36	29.6
1339	0.4787	0.3286	2.583	1397.76	5	4053.22	24.6
1271	0.4252	0.2922	2.690	1514.54	5.5	5032.84	31.9
1188	0.3661	0.2666	2.644	1687.91	6	4306.65	26.8
1134	0.321	0.2386	2.695	1923.22	6.5	4872.13	30.9
1069	0.2902	0.224	2.643	2025.55	7.5	4553.93	28.3
1027	0.2572	0.2065	2.584		8		
976	0.2436	0.2003	2.520		8.5		
			⟨d⟩ 1657.58 ***exp 1689 nm***				

Table III

Calculated optical properties by Swanepoel method for CdTe thin films (sample 21)

λ, nm	**T_M**	**T_m**	**n**	**d_1, nm**	**m**	**α, cm^{-1}**	**σ_{opt}, 10^{11}**
2498	0.9441	0.5529	2.382				
2181	0.9362	0.5474	2.391				
1935	0.914	0.5506	2.353	1403.159	3	64.44	2.85
1752	0.8929	0.5377	2.372	1442.819	4	511.03	2.53
1596	0.8624	0.5302	2.358	1414.053	4.5	455.21	6.75
1474	0.8305	0.5024	2.420	1437.777	5	1185.00	5.06
1363	0.7756	0.4869	2.397	1316.820	5.5	896.46	11.6
1277	0.726	0.4498	2.479	1467.810	6	1981.87	9.55
1192	0.66	0.4287	2.451	1481.673	6.5	1656.57	106
1129	0.5966	0.3158	3.043		7.5	1480.10	5.8
1064	0.541	0.3742	2.457	1473.072	8	1005.82	15
1016	0.4881	0.3383	2.539	1547.714	8.5	2523.31	18
965	0.4509	0.3252	2.490	1444.584	9.5	3076.79	22.6
928	0.4095	0.2977	2.548	1422.981	10.5	3766.45	19.7
889	0.3759	0.2835	2.500	1403.159	11.5	3346.23	
			⟨d⟩ 1441.13 ***exp 1485 nm***				

Table IV

Calculated optical properties by Swanepoel method for CdS/CdTe heterojunction (sample 24)

λ, nm	**T_M**	**T_m**	**n**	**d_1, nm**	**m**	**α, cm^{-1}**	**$σ_{opt}$, 10^{11}**
1804	0.3662	0.2589	2.745				
1611	0.3907	0.2698	2.758				
1434	0.4132	0.2783	2.781	1196.811	3.5	5683.348	37.2
1304	0.4402	0.2983	2.699	1396.410	4	3771.711	24
1188	0.4758	0.3073	2.763	1293.906	4.5	4733.311	30.8
1102	0.5022	0.3264	2.692	1341.083	5	3214.134	20.4
1023	0.5409	0.3457	2.666	1781.445	6	2375.072	14.9
961	0.6244	0.3783	2.665	1516.782	6.5	2219.331	13.9
			⟨d⟩ 1421.071 exp 1490 nm				

Table V

Calculated optical properties by Swanepoel method for CdTe thin films (sample 24)

λ, nm	**T_M**	**T_m**	**n**	**d_1, nm**	**m**	**α, cm^{-1}**	**$σ_{opt}$, 10^{11}**
2477	0.885	0.5265	2.402				
2066	0.8812	0.5172	2.432				
1782	0.8764	0.5191	2.419	1290.680	2.5	571.4192	3,25
1566	0.8664	0.5077	2.449	1293.241	3	1040.131	5,99
1397	0.8549	0.5069	2.436	1292.578	3.5	724.5566	4,15
1268	0.8444	0.4914	2.484	1265.469	4	1369.256	8
1159	0.826	0.4907	2.461	1319.135	4.5	808.1503	4,68
1073	0.8111	0.4724	2.516	1294.507	5.5	1637.885	9,7
998	0.7767	0.4691	2.478	1391.304	6	972.2801	5,67
939	0.7573	0.4466	2.550	1350.514	7	2085.314	12,5E
888	0.6826	0.4379	2.452	1792.857	8	947.8748	5,47
850	0.6309	0.4286	2.380		9		
			⟨d⟩ 1365.59 exp 1215 nm				

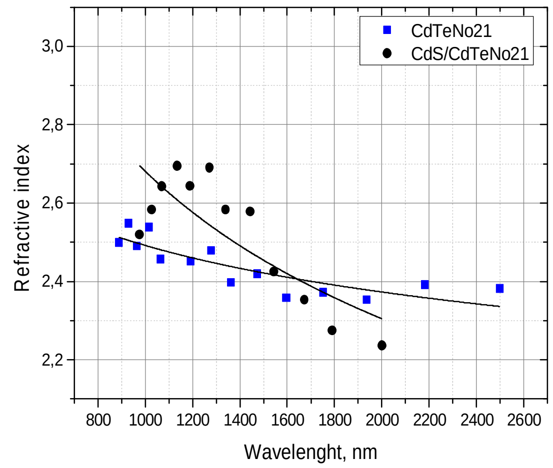

Fig. 4. Refractive index versus wavelength of CdTe thin film and heterojunction of CdS/CdTe (sample 21).

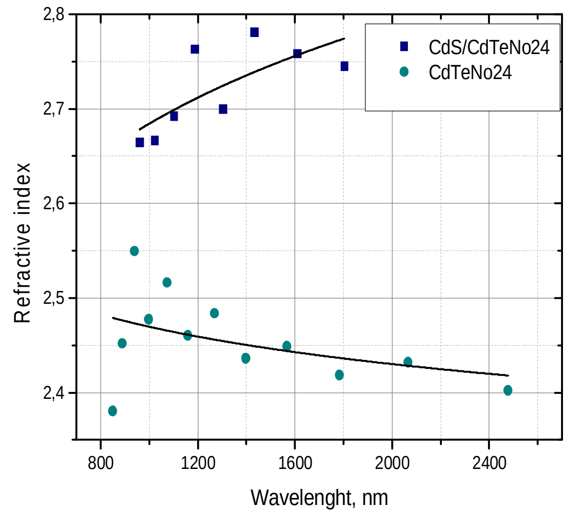

Fig. 5. Refractive index versus wavelength of CdTe thin film and heterojunction of CdS/CdTe (sample 24).

$$m = \left(\frac{\lambda_2}{\lambda_1 - \lambda_2}\right), \qquad (14)$$

where λ_1 and λ_2 are the wavelengths of two adjacent transmission maxima ($\lambda_1 > \lambda_2$).

For a region where is a strong absorption of light, the refractive index is determined as follows:

$$\alpha = \frac{1}{d} \ln \frac{(n-1)^3 (n-s^2)}{E_m - (E_m^2 - (n^2-1)^3 (n^2 - s^4))^{0.5}}, \qquad (15)$$

where

$$E_m = \left(\frac{8n^2 s}{T_m}\right) - (n^2-1)(n^2-s^2), \qquad (16)$$

For heterojunction CdS/CdTe takes place a significant increase in the absorption coefficient of light several times, primarily in the short-wave region of the spectrum (Fig. 6-7). This is due to the fact that the thin layer of CdS thanks to the large band gap (2.42 eV) plays the role of an «absorption window» for absorbing light.

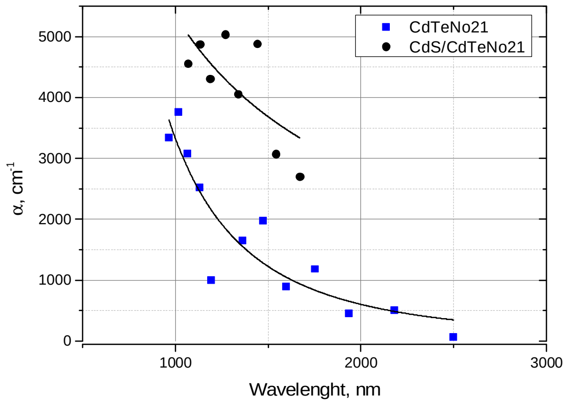

Fig. 6. Absorption coefficient versus wavelength of CdTe thin film and heterojunction of CdS/CdTe (sample 21).

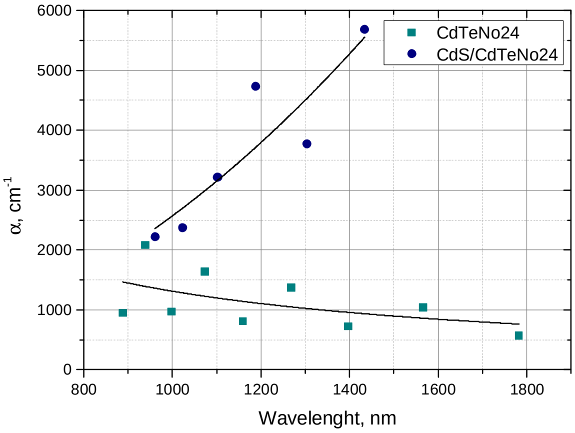

Fig. 7. Absorption coefficient versus wavelength of CdTe thin film and heterojunction of CdS/CdTe (sample 21).

The photons absorbed in the window layer do not contribute to the photocurrent, as recombination is very likely to occur, resulting in scattering of light. Therefore, absorption in the CdS layer is a source of significant loss.

For samples 21 and 24, a significant difference in absorption coefficients is observed for the corresponding wavelengths. It can be noted that the absorption coefficient for thin films of CdTe acquires larger values than for the CdS /CdTe heterojunction at the corresponding wavelengths for both specimens.

Conclusions

1. CdS/CdTe heterojunction on glass substrates are deposited by the method of open evaporation in a vacuum for various technological factors, including different thicknesses.
2. An analysis of the optical properties of thin films of CdTe was carried out and their change after the addition of an "absorption window" of CdS was investigated.

3. It was found that the thin layer of CdS significantly increases the absorption properties of the film.
4. The thickness of the film is theoretically calculated and the results obtained coincide with the experimental studies of the profilometer.
5. It is shown that CdS / CdTe heterojunction due to their high absorption capacity have the prospect of using as photovoltaic light converters.

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Оптичні властивості гетероструктури CdS / CdTe, отримані методом фізичного осадження з парової фази

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У статті наведено дослідження оптичних властивостей тонкого шару сульфіду кадмію в плівках телуриду кадмію. Тонкі плівки CdTe були отримані методом відкритого випаровування у вакуумі, використовуючи різні технологічні фактори, зокрема, різну товщину (різний час осадження τ) на скляних підкладах. Після осадження оптичні властивості аналізували методом Swanepoel, використовуючи спектри пропускання. Наступний тонкий шар CdS осаджувався методом термічного випаровування на тонких плівках CdTe. Досліджено зміну оптичних властивостей гетероструктури CdS/CdTe у порівнянні з тонкими плівками CdTe. Використовуючи метод Swanepoel, розраховано основні оптичні константи, такі як показник заломлення, коефіцієнт поглинання та оптична провідність. За допомогою цього методу отримано товщину тонкої плівки та порівняно її з експериментальними значеннями, отриманих за допомогою профілометра.