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Structure and Optical Properties of CdTe and CdS Thin Films after Hard Ultraviolet Irradiation

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The influence of hard ultraviolet radiation on the crystalline structure, surface morphology and optical characteristics of CdS and CdTe semiconductor layers obtained by direct current magnetron sputtering are investigated. It was established that the optical characteristics of the studied films CdS and CdTe are insensitive to hard ultraviolet irradiation. The crystalline structure of the CdS and CdTe layers is changed after irradiation. The period of the lattice for cadmium sulfide films increases from c = 6.77(01) Å to c = 6.78(88) Å, which may be due to the formation of point defects and defective complexes. Decrease the integral FWHM of the peaks on the X-ray diffraction patterns of the layers of CdS and CdTe was observed, due to the increase of the coherent scattering regions as a result in the process of near-surface layers partial recrystallization of the investigated films.

Keywords: cadmium telluride, cadmium sulfide, non-pulsed direct current magnetron sputtering, hard ultraviolet, thin films.

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Introduction

The CdTe/CdS thin film layers heterosystem is promising for the creation of economical high-performance film solar cells for terrestrial and space usage [1-4]. At present, the value of the efficiency of the real photovoltaic converters obtained on the basis of this heterojunction is lower than the theoretically possible [5]. This is due to the high specific resistance of the base layer of cadmium telluride, the low lifetime of minority carriers in this material, the low quality of separation barrier and the inadequate use of new physical principles for the solar cells design. For example, the creation of varieussed structures in the area of the separation barrier allows us to improve the photoelectric converters' parameters [6]. Direct current magnetron sputtering (DC magnetron sputtering) is one of the most economical and high-tech methods for obtaining thin films which are used in various microelectronic devices. Technological problems caused by low conductivity of pulsed pressed semiconductor targets and relatively low emissivity of materials for cadmium sulfide and cadmium telluride were solved in [7].

Sunlight in space at the top of Earth's atmosphere is called extraterrestrial solar irradiance. A short-wave (100 - 279 nm) hard ultraviolet light (UV) is completely absorbed by the ozone layer and atmosphere. With the usage of solar cells based on the CdTe/CdS heterosystem in outer space, the radiation of hard ultraviolet can cause a degradation of the solar cells' output parameters.

The crystalline structure and optical properties of the semiconductors layer in solar cells based on the CdS/CdTe film heterosystems significantly affect the separation barrier quality and the solar cell's initial parameters. The reason for this may be the change in the material properties of the CdS window layer and the CdTe base layer under the action of external irradiance. Therefore, the study of the influence of hard ultraviolet radiation on the structure and optical properties of CdS and CdTe films obtained by DC magnetron sputtering for space solar cells is relevant.

I. Experiments

CdS and CdTe thin films were condensed by DC magnetron sputtering on soda-lime glass substrates [7]. Physical and technological modes for CdS films were obtained at: substrate temperature T_{sub}= 150 – 160 ^{0}C, pressure of inert gas Ar P_{Ar}= 0,9 Pa, magnetron discharge current I = 40 mA, the voltage on magnetron V = 300 - 340 V, deposition time 10 min, substrate-target distance 3 cm. Physical and technological modes for CdTe films were obtained at: T_{sub}= 280 – 320 ^{0}C, P_{Ar} = 0.9 Pa, I = 80 mA, V = 430 - 470 V, deposition time 12 min, substrate-target distance 3 cm.

Taking of X-ray diffractograms (XRD) for the CdS and CdTe films was carried out by θ-2θ scanning method using X-ray diffractometer DRON-4 Kα-radiation of a molibdenium anode. The morphology of the surface layers of CdTe was investigated on a scanning electron microscope TESCAM-VEGA3.

Optical studies of semiconductors layers (transparency and reflection spectra) were conducted using the spectrometer SF-2000. The transmission spectrum of studied films was used to determine the thickness of the layers. The thickness of the layers was determined by the formula:

$$t = \frac{M \cdot l_1 \cdot l_2}{2\left(n(l_1) \cdot l_2 - n(l_2) \cdot l_1\right)} \qquad (1)$$

where λ_1, λ_2 – the wavelengths of two adjacent extremums (interferential maxima or minima of transmission spectrum) in nm; $n_{\lambda1}$, $n_{\lambda2}$ – refractive index, depending on the wavelength λ_1, λ_2.

The bandgap of thin films was determined by calculating the dependence of absorption coefficient on the wavelength α(λ) using:

$$T = (1 - R) \cdot e^{-a \cdot t}, \qquad (2)$$

where *T* - transmission coefficient; *R* - reflection coefficient; ***t*** - film thickness.

The CdS and CdTe polycrystalline films bandgaps were determined by extrapolation of the linear portion of the $(\alpha \cdot h\nu)^2 = f(h\nu)$ curves (where ***h*** - Planck constant, *ν* - frequency) to the intersection with the hν energy axis.

Cadmium sulfide and cadmium telluride films were irradiated by hard ultraviolet with the energy of quanta 10 eV for 10 hours. The irradiation was carried out using an argon barrier lamp with vacuum ultraviolet radiation with a wavelength main mode of 125 nm. The maximum energy illumination in the window plane of the radiation source corresponded to the value of 10^{20} - 10^{21} quanta/m^2*s. The area of irradiated samples is 1.5 cm^2.

II. Results and discussion

The XRD patterns of CdS films in the initial state and after hard UV irradiation (CdS+UV) are shown in figure 1.

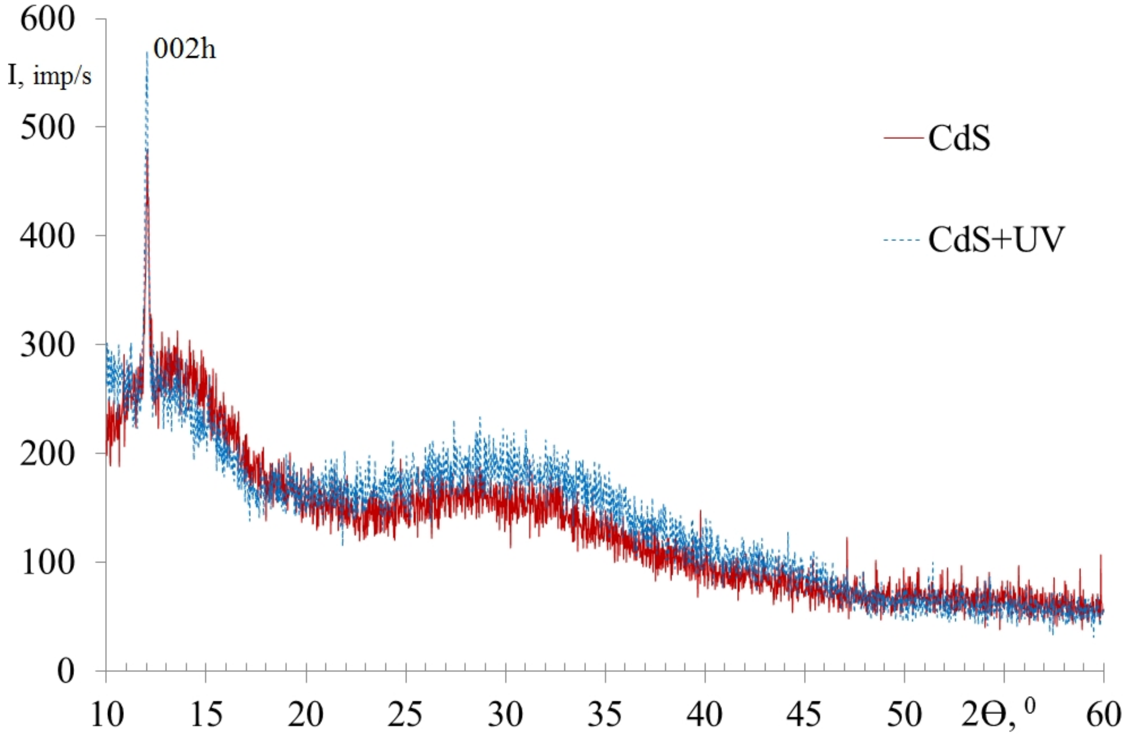

Fig. 1. The XRD patterns of CdS films in the initial state and after hard UV irradiation (CdS+UV).

Table 1

The results of the XRD analysis of CdS films in the initial state and after hard UV irradiation (CdS + UV)

	hkl	Peak position, °	Interplanar spacing, Å	Intensity, imp/s	FWHM, °	D, nm	$\Delta d/d*10^{-3}$, a.u.
CdS	002	12.03	3.385	145	0.24	15	7.5
CdS+UV	002	11.99	3.394	208	0.20	18	10

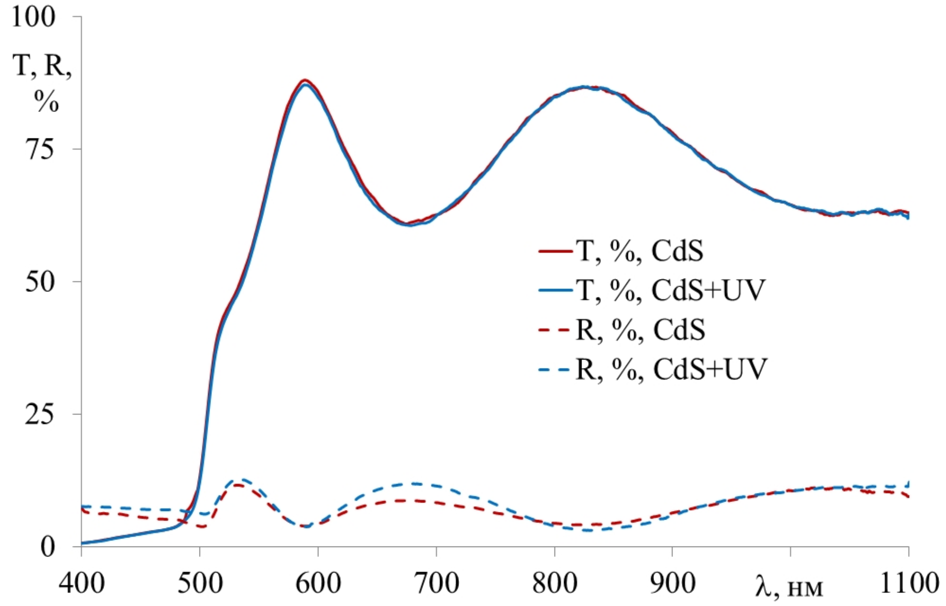

Fig. 2. Optical studies of semiconductors layers transparency and reflection spectra of CdS films in the initial state and after hard UV irradiation (CdS+UV).

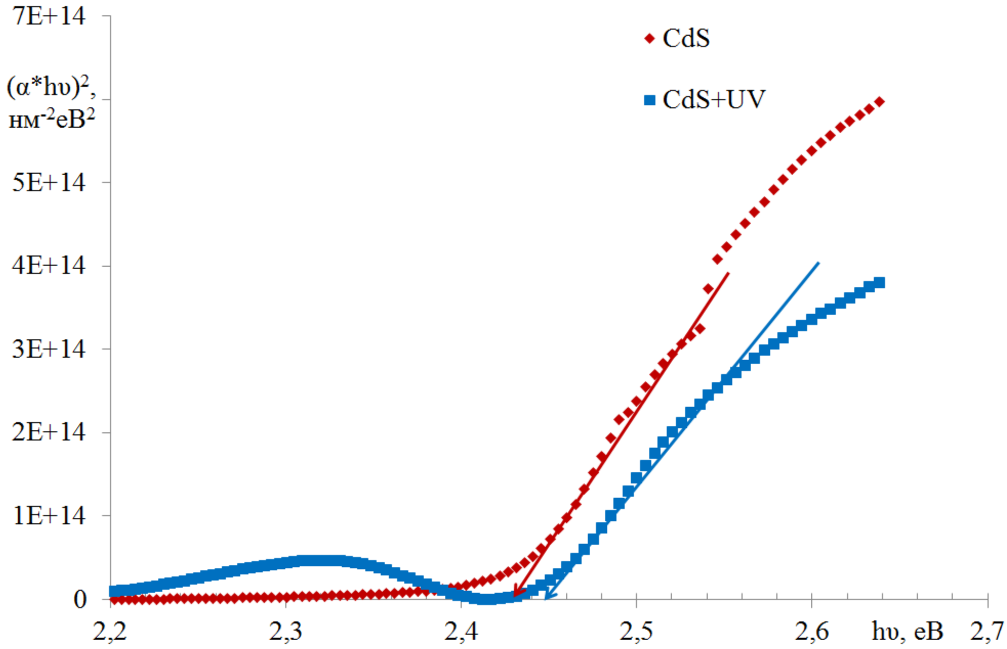

Fig. 3. Dependences of the $(\alpha \cdot h\nu)^2 = f(h\nu)$ curves of CdS films in the initial state and after hard UV irradiation (CdS+UV).

The results of the XRD analysis performed for a CdS stable hexagonal phase are shown in table 1. The reflection of the peak (002) on the angle 12.03^0 was found. The calculated constant of crystal lattice *c* for the sample in the initial state is *c* = 6.77(01) Å, which is 0.74% different from the tabulated value for hexagonal cadmium sulfide (PCPDFWIN # 41-1049, *a* = 4.14092 Å, *c* = 6.7198 Å). After hard UV irradiation of the cadmium sulfide thin film layer the peak reflection of the stable hexagonal phase - (002) on the 11.99^0, respectively, was detected. Calculated crystal lattice constant c = 6.78(88) Å, which is 1.03 % different from the table value. The integral full width at half maximum (FWHM) of the captured peak for the initial state decreases by from 0.24 degrees at the initial state to 0.2 degrees after UV irradiation.

The results of optical studies, shown in the figure 2, say that CdS films average transparency coefficient in the initial state and after irradiation is 85 %. Calculated average reflection coefficient is n = 2.34 - 2.51, thickness of obtained CdS layer is t = 360 nm. The bandgap is Eg = 2.42 eV. After hard UV irradiation of the cadmium sulfide thin film the spectral dependences were not changed. Average values of reflection coefficient n and Eg for irradiated by hard UV samples are similar to the corresponding values of not-irradiated samples of CdS thin films. Dependences of the $(\alpha \cdot h\nu)^2 = f(h\nu)$ curves of CdS films are shown in the figure 3.

The XRD of CdTe films in the initial state and after hard UV irradiation are shown in figure 4. The XRD spectrum analysis of CdTe layer was performed for metastable hexagonal phase with reflection of the peak (201) at the angle 21.64°. The reflexes (002) and multiplies of it (006) and (008). The calculated constants of crystal lattice are a = 4.50(73) Å and c = 7.52(47) Å (PCPDFWIN #19-0193, a = 4.58 Å, c = 7.50 Å). After irradiation of the CdTe film it was found, that the intensity of the reflection peak (201) increased, while the intensity of all other peaks decreased. At the same time, the integral FWHM of all peaks decreased. The calculated values of permanent crystalline lattice constant for CdTe were similar to these values in the initial state. Figure 5 shows the cadmium telluride films surfaces morphology before and after hard UV irradiation. After irradiation on the surface of the CdTe layers, there are accumulated crystalline grains whose sizes exceed the grain size of the films in the initial state.

Figure 6 shows transmission and reflection spectra of cadmium telluride films before and after hard UV irradiation. The results of optical studies indicate that in the infrared spectral region, the average transparency coefficient of the CdTe films in the initial state is 65 %. The parameters for the CdTe film are calculated: n = 2.31 - 2.72, t = 6.2 μm, Eg = 1.52 eV. Thus, after hard UV irradiation of the cadmium telluride base layers, the spectral dependence of the transparency coefficient of cadmium telluride films does not change, as case in the CdS films. The mean values of the refractive index n and the bandgap of material Eg, both for the CdS layers and for the CdTe layers, do not differ from the values of

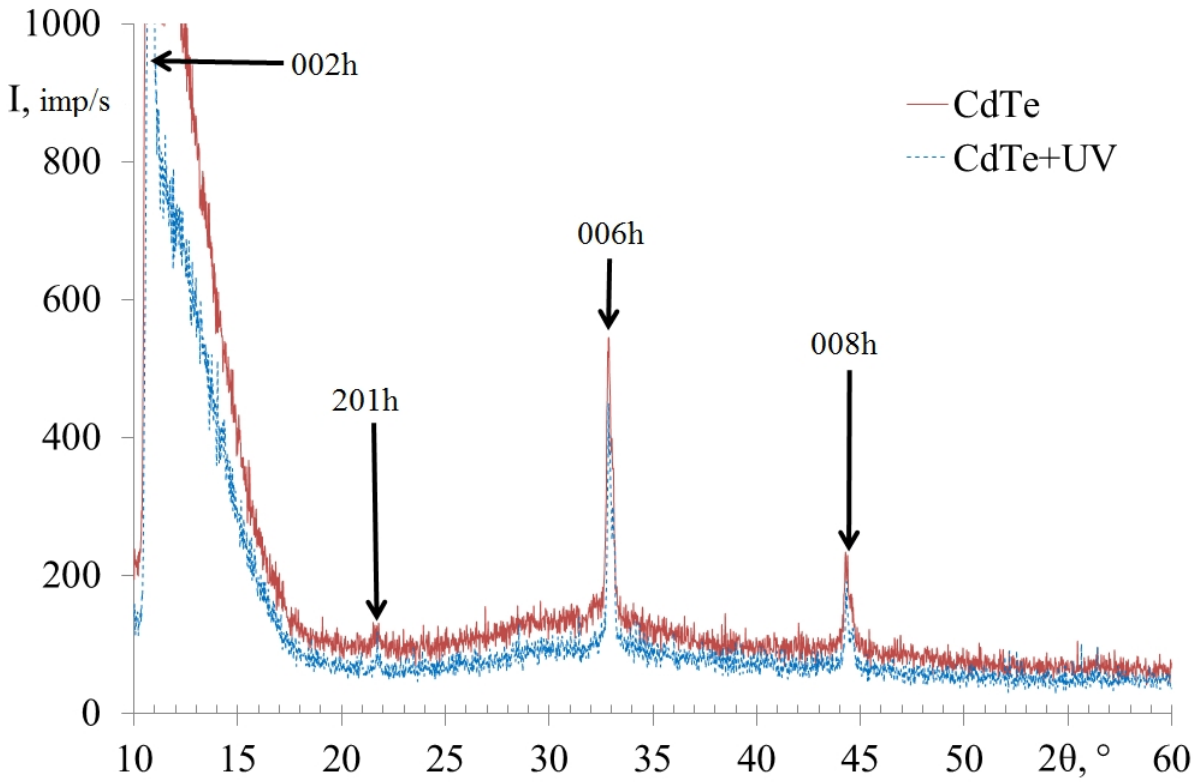

Fig. 4. The XRD patterns of CdTe films in the initial state and after hard UV irradiation (CdTe+UV).

Table 2

The results of the XRD analysis of CdTe films in the initial state and after hard UV irradiation (CdTe+UV)

	hkl	Peak position, °	Interplanar spacing, Å	Intensity, imp/s	FWHM, °	D, nm	$\Delta d/d*10^{-3}$, a.u.
CdTe	002	10.77	3.777	10306.77	0.195	19	7.2
	201	21.64	1.889	12.52	0.41	9	16
	006	32.85	1.254	375.23	0.25	16	4.1
	008	44.31	0.94	117.47	0.31	13	3
CdTe+UV	002	10.81	3.766	7636.56	0.16	23	4.3
	201	21.71	1.883	22.76	0.14	26	19
	006	32.88	1.253	304.71	0.23	16	3
	008	44.33	0.94	96.22	0.26	15	2.6

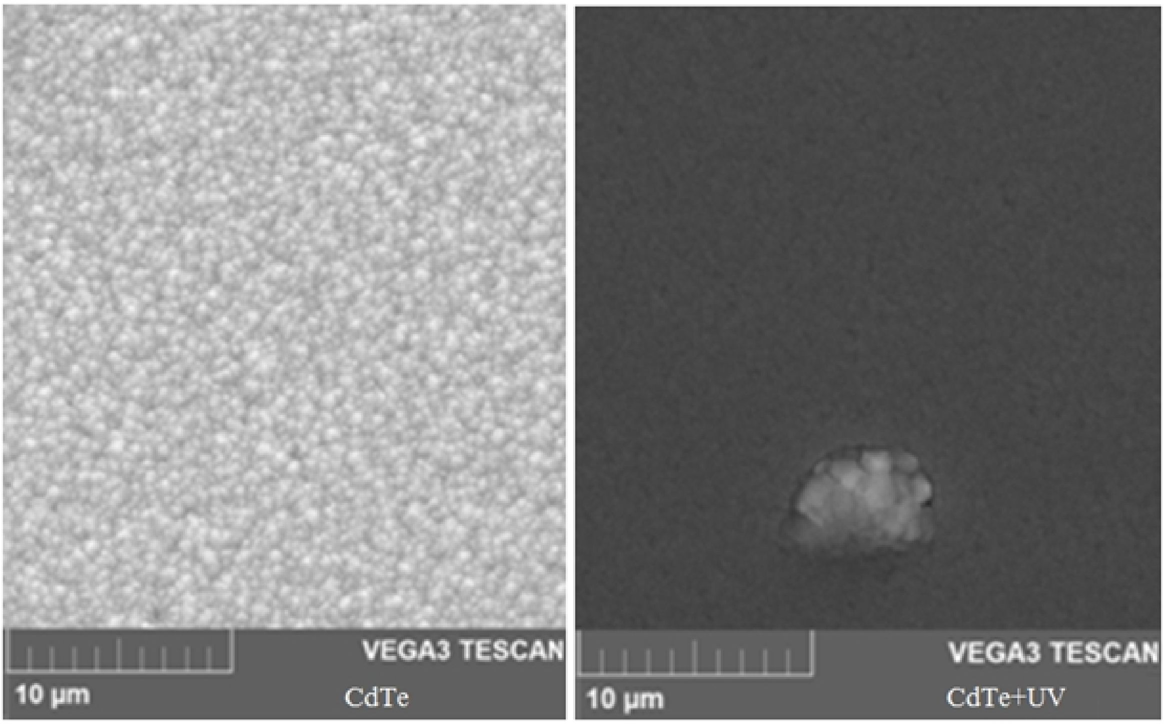

Fig. 5. Morphology of CdTe films surface in the initial state and after hard UV irradiation (CdTe+UV).

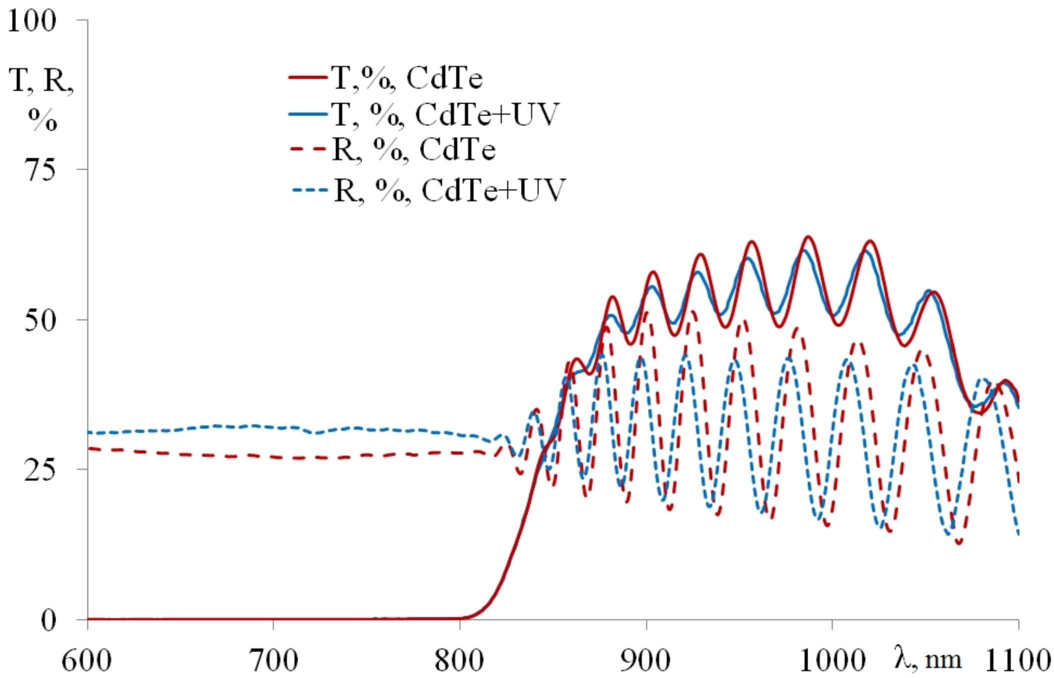

Fig. 6. Optical studies of semiconductors layers transparency and reflection spectra of CdTe films in the initial state and after hard UV irradiation (CdTe+UV).

these optical parameters before irradiation.

Conclusions

The influence of hard ultraviolet radiation on the crystalline structure, surface morphology and optical characteristics of CdS and CdTe semiconductor layers obtained by direct current magnetron sputtering were investigated.

It was established that the optical characteristics of the studied films CdS and CdTe are insensitive to hard ultraviolet irradiation. The transparency of films of cadmium sulfide in the visible wavelength range is 85%, which allows the use these films as window layers in the solar cells based on the CdS/CdTe heterostructure.

The crystalline structure of the CdS and CdTe layers was changed after irradiation. The period of the lattice for cadmium sulfide films increases from *c* = 6.77(01) Å to *c* = 6.78(88) Å, which may be due to the formation of point defects and defective complexes.

As a result of hard UV irradiation, a decrease the integral FWHM of the peaks on the X-ray diffraction patterns of the layers of CdS and CdTe was observed, due to the increase of the coherent scattering regions D as a result in the process of near-surface layers partial recrystallization of the investigated films.

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Вплив жорсткого ультрафіолету на структуру та оптичні властивості шарів CdS та CdTe

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Досліджено вплив жорсткого ультрафіолетового випромінювання на кристалічну структуру, морфологію поверхні та оптичні характеристики напівпровідникових шарів CdS та CdTe, отриманих магнетронним розпиленням на постійному струмі. Встановлено, що оптичні характеристики досліджених плівок CdS та CdTe нечутливі до опромінення жорстким ультрафіолетом. Кристалічна структура шарів плівок CdS і CdTe після опромінення змінюються. Період ґратки для плівок сульфіду кадмію збільшується від c = 6,77(01) Å до c = 6,78(88) Å, що може бути пов’язано з утворенням точкових дефектів та дефектних комплексів. В результаті опромінення жорстким ультрафіолетом спостерігається зменшення ширини піків на рентгендифрактограмах шарів CdS і CdTe, що пов’язано зі збільшенням областей когерентного розсіювання в результаті часткової рекристалізації приповерхневих шарів досліджених плівок.

Ключові слова: телурид кадмію, сульфід кадмію, неімпульсне магнетронне розпилення на постійному струмі, жорсткий ультрафіолет, тонкі плівки.