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Effect of Substrate Temperature on the Structural Properties of $Cd_xZn_{1-x}Te$ Films Grown by Close-Spaced Sublimation Method

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In this work by energy dispersive analysis of X-rays, scanning electron microscopy and X-ray diffraction methods films of $Cd_xZn_{1-x}Te$ solid solution, obtained by a close-spaced vacuum sublimation technique under different temperatures of glass substrate, has been studied. Films were deposited by the co sublimation of Cadmium Telluride (CdTe) and Zinc Telluride (ZnTe) chunks, mixed in the ratio of 2:1. The effect of substrate temperature on the surface morphology, elemental and phase composition, lattice parameter, scattering domain sizes has been studied. The results of these studies can be used for obtaining absorber layers of tandem solar cells, basic layers of X-ray and gamma detectors.

Keywords: CdZnTe, Closed space sublimation, XRD, Bandgap, Film.

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1. INTRODUCTION

Chlorine doped Cadmium Telluride CdTe:Cl single crystals were used as basic material for X-ray and gamma-ray detectors during a long period [3]. However, recent time a trend of replacing this material by solid three-component solutions, especially of Zn-containing, has observed. This is due to a number of significant advantages of $Cd_xZn_{1-x}Te$ solid solutions over the two-component compound, namely: higher resistivity of the material, higher atomic binding energy, tunable band gap of semiconductor by adjusting the film composition [11].

Last time mono- and polycrystalline films of three-component solution with high-quality crystal structure are used as a detector material [5]. Wherein adjusting of Zn constitution allows to vary band gap of the material in the range from E_{g1} = 1.50 eV (CdTe) to E_{g2} = 2.26 eV (ZnTe). The films of $Cd_xZn_{1-x}Te$ with band gap in the range of 1.65-1.75 eV are perspective material for absorber layers of X-ray and gamma-ray detectors and tandem solar cells that can operate at room temperature [6].

There are several techniques for preparation of $Cd_xZn_{1-x}Te$ films, such as electrodeposition [24], molecular beam epitaxy [19], metal-organic chemical vapor desposition [20], sputtering [2], thermal vacuum evaporation [20].We used close-spaced vacuum sublimation (CSVS) method for the deposition of solid solutions. In comparison with other techniques, close spaced sublimation is quite simple and cheap method, which allows to obtain films in conditions close to thermodynamically equilibrium, where structurally perfect layers of chalcogenides are grown [6]. In case of using CSVS method, properties of the films depend on physical and technological conditions of their growing. According to the analysis of published data [6], substrate temperature has the greatest effect on structural, optical and electrophysical properties of obtained layers. Thus the aim of this work is to investigate effect of substrate temperature on structural and substructural properties of $Cd_xZn_{1-x}Te$ films obtained by close-spaced vacuum sublimation.

2. EXPERIMENTAL DETAILS

Films of $Cd_xZn_{1-x}Te$ solid solutions were deposited on non-oriented glass substrates by close spaced vacuum sublimation in vacuum equipment VUP-5M. Residual gas pressure in the chamber did not exceed of 5×10^{-3} Pa. Evaporator temperature was T_e = 923 K, substrate temperature was varied in the range of T_s = 673-823 K. Two different sources (CdTe and ZnTe mixed in the ratio 2:1) were co-evaporated to form films.

The surface morphology of the films has been investigated by optical and scanning electron microscopy (SEM). The average grain size (D) in the layers was estimated by Jeffries method [16].

Elementary composition of the films was determined by X-ray energodispersive spectroscopy (EDAX) using the console to the electron microscope. Determination of the mass concentration of the elements, that are included in film (C_{Cd}, C_{Zn}, C_{Te}), was carried out at least in 3 points on the surface of samples, following averaging of result was performed.

Structural investigations of the films were performed with an X-ray diffractometer, DRON 4-07 (λ = 0.15406 nm, U = 40 kV, I = 40 uA), with Cu K_α radiation over the range 20° ≤ 2θ ≤ 80° (where 2θ is the Bragg angle) at room temperature.

The diffraction patterns obtained under study were normalized to the intensity of (111) peak of the cubic phase. Phase analysis was done by comparison of interplanar distances and relative intensities from the

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investigated samples and references according to Joint Committee on Powder Diffraction Standards (JCPDS card № 01-089-1397).

Lattice constants a of cubic phase were found by the position of the $K_{\alpha 1}$ component of the diffraction pattern observed at large angles from the following equation

$$a = \frac{\lambda}{2\sin\theta}\sqrt{(h^2 + k^2 + l^2)} \quad (2)$$

Subsequently, the values of these constants was clarified using the the Nelson–Riley extrapolation method [15]. Thus plots were built in $a(c) - 1/2\cos^2\theta(1/\sin(\theta)+1/\theta))$ coordinates. Linear approximation of obtained points was conducted using the method of least squares using the software package OriginPro.

Average coherent scattering regions (CSR) size was determined from the Debye-Scherrer formula:

$$L = \frac{k \cdot \lambda}{\beta \cdot \cos\theta}, \quad (4)$$

Where λ is the x-ray wavelength, β is the line width of the “pure” diffraction profile resulting from small crystallite size, and k is a constant approximately equal to unity and related to crystallite shape ($k = 0.9$).

Detailed methodology for determining the structural characteristics of the films is described in [15].

3. RESULTS AND DISCUSSION

In figure 1 surface morphology of the films grown under different substrate temperatures is shown.

As it is seen from figure, average grain sizes in films depends on technological conditions of growing and increases with increasing the substrate temperature T_s. At T_s = 673 K it is D = 4.1 microns, while at T_s = 823 K - D = 14.5 microns. Particularly significant increase of grain size of $Cd_xZn_{1-x}Te$ films is observed at T_s > 700 K (figure 1). This can be explained by changing of their deposition regime from the molecular to the gas-dynamic and approaching of growth conditions close to thermodynamically equilibrium [15].

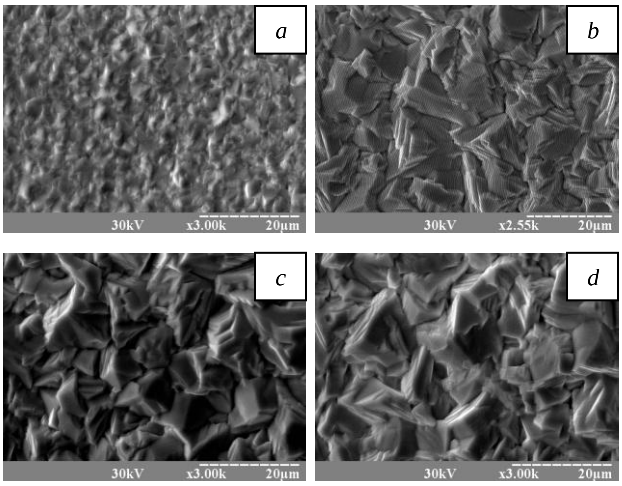

Fig. 1 – SEM images of surface morphology of the $Cd_xZn_{1-x}Te$ films, obtained on non-oriented glass substrates under different substrate temperatures T_s, K: 673 (a), 723 (b), 773 (c) and 823 (d).

In figure 2 typical EDAX spectras of syntezed layers are shown. The analysis shows that the film includes only components of a solid solution - Cd, Zn, Te. According to EDAX, films contain 7-13 at. % of Zinc. Extraneous components that belong to substrate or residual atmosphere of the vacuum chamber, were not identified.

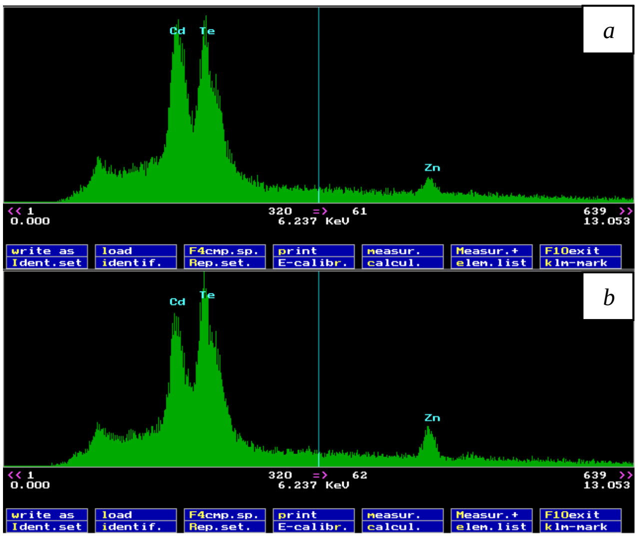

Рис.2. - Typical EDAX spectra of films obtained under different substrate temperature T_s, K: 723 (a) and 823 (b).

The XRD patterns of the $Cd_xZn_{1-x}Te$ films obtained at different substrate temperatures are presented in Figure 2. In these patterns positions of diffraction peaks from CdTe (solid black line) and ZnTe (dashed red line) compounds are shown. As it is seen on figure 2, reflection from planes of solid solution locates between reflections from clear materials. This indicates that we invistigated $Cd_xZn_{1-x}Te$ films.

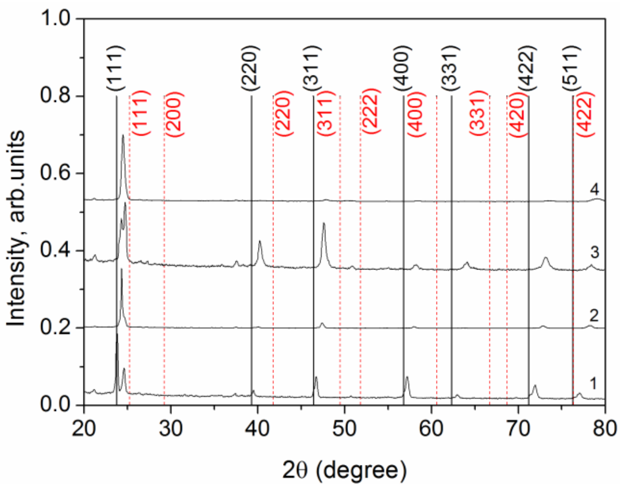

Fig. 3 – Diffraction patterns of $Cd_xZn_{1-x}Te$ films obtained under different substrate temperature T_s, K: 673 (1), 723 (2), 773 (3), 823 (4). Vertical lines correspond to JCPDS reference data of CdTe (solid line) and ZnTe (dashed line) compounds.

Phase analysis of samples was performed using JCPDS directory (card № 01-089-1397). As it is seen from figure, peak at angles 24.10°-24.60° dominates, which corresponds to the reflection from the (111) plane of the cubic phase $Cd_xZn_{1-x}Te$. In some cases, there was a double peak, indicating the formation of two solid solutions with different concentrations of zinc. But basically, the samples were single-phase and contained cubic phase. Oxide and other extraneous phases in the condensates were found.

The lattice parameters of A_2B_6 compound semiconductors are very sensitive to changes in the material stoichiometry, impurity inclusions, oxidation, etc., what is why precise measurement of this quantity makes it possible to study these processes. We carried out X-ray diffraction (XRD) determination of the lattice parameter for the material of films obtained under different regimes of condensation. As studies have shown, the lattice parameter of the material film was a = 0.63166 - 0.64144 nm.

In Figure 4 the dependence of the lattice parameter a under the substrate temperature is shown. As it is shown in Fig. 4, as the substrate temperature T_s increases from 673 K to 823 K, the calculated values of lattice parameter a of film material decreases from a = 0.64144 nm to a = 0.63166 nm. This may indicate an increase of zinc content in a high-temperature condensates because atomic radius of zinc atom (142 pm) is smaller than cadmium (161 pm).

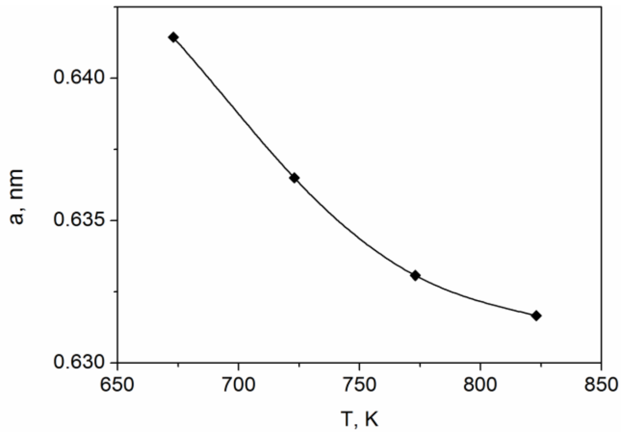

Fig. 4 – Dependence of the lattice parameter a of $Cd_xZn_{1-x}Te$ films on substrate temperature.

Results of calculation of CSD sizes in $Cd_xZn_{1-x}Te$ films in directions perpendicular to (111), (220) and (311) crystallographic planes are shown in Figure 5. It is found that these dimensions take the following values: $L_{(111)}$ = 17-31 nm, $L_{(220)}$ = 16-32 nm, $L_{(311)}$ = 12-27 nm. As it is seen in figure, with the increase of substrate temperature from 673K to 723K CSR size, for example in direction (111), increases slightly from 26 to 31 nm, but with further increase of T_s it desreases to 17-21 nm. A similar trend is observed for the CSR size in all other crystallographic directions. Similar L - T_s dependence with a maximum at temperatures 600-700 K was observed earlier in A_2B_6 compounds films [16]. Deterioration of structure of the films after increase of substrate temperature above 673 K can be explained by re-evaporation of components of solid solution (especially of cadmium) from the surface of the condensate, which leads to occurrence of additional dislocations in their volume and leads to a reduction in the CSR sizes.

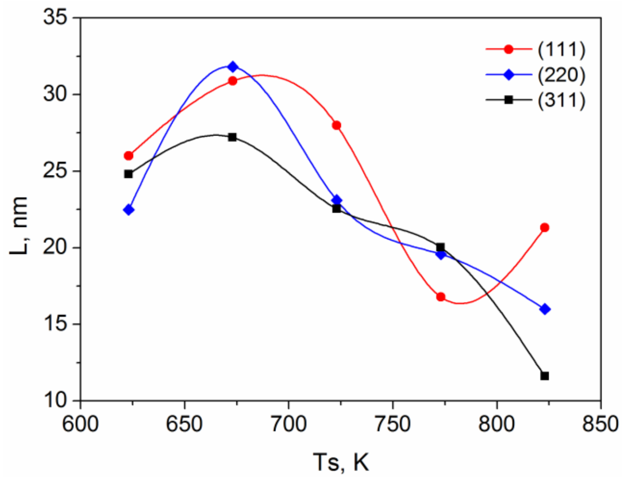

Fig. 5 – Dependence of CSR sizes *(L)* of $Cd_xZn_{1-x}Te$ films on substrate temperature. Values for the crystallographic directions [111], [220] and [311] are presented.

According to the results of the studies, due to its structural and substructural features, obtained $Cd_xZn_{1-x}Te$ films can be used as an absorbing layers of tandem solar cells and as basic layers of X-ray detectors and gamma-ray detectors. Thus films grown at substrate temperatures close to 723 K have optimal for instrumental usage properties. Such films have single-phase structure with sufficiently large grain size and high crystalline quality.

4. CONCLUSION

In this work by energy dispersive analysis of X-rays, scanning electron microscopy and X-ray diffraction methods films of CdxZn1-xTe solid solution, obtained by a close-spaced vacuum sublimation technique under different temperatures of glass substrate, has been studied. The effect of substrate temperature on the surface morphology, elementary and phase composition, lattice parameter, scattering domain sizes has been studied.

It is shown that obtained films have a polycrystalline structure with a grain size of 4-15 microns, which increases with increasing of the substrate temperature. Films were mostly single-phase and contained a cubic phase of $Cd_xZn_{1-x}Te$.

It was determined that the experimental values of the lattice parameter of the material of the films decreases from a = 0.64144 nm to a = 0.63166 nm as substrate temterature T_s increases from 673K to 823K, which may indicate an increase of zinc content in a high-temperature condensates. CSR sizes in films take following values: $L_{(111)}$ = 17-31 nm, $L_{(220)}$ = 16-32 nm, $L_{(311)}$ = 12-27 nm, thus L-T_s dependences have form of the curve with a maximum at substrate temperature T_s = 673K.

Obtained $Cd_xZn_{1-x}Te$ films can be used as an absorbing layers of tandem solar cells and as basic layers of X-ray detectors and gamma-ray detectors.

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