STRUCTURAL AND OPTICAL PROPERTIES OF ZnTe THIN FILMS

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Abstract*–Thin films of ZnTe have been prepared by close spaced sublimation technique. The deposited films have been characterized by using optical absorption, X-ray diffraction (XRD) and scanning electron microscopy (SEM). Structural investigations performed by X-ray diffraction technique showed that studied samples are polycrystalline and have a cubic (zinc blende) structure. XRD patterns have been used to determine the microstructural parameters (crystallite size, lattice parameter) of investigated films. Surface morphology studies SEM shows that the grains are uniformly distributed over the entire surface of the substrate. Optical properties of ZnTe films were studied extensively in the range of incident photon energy (0.5-4.0) eV. In the studied ZnTe films the direct transitions take place.*

Keywords: *ZnTe thin films, structural properties, optical properties.*

1.INTRODUCTION

Zinc telluride (ZnTe), as a direct semiconductor with a band gap of 2.28 eV at T=300 K, is an important component of the II-VI family and an attractive material for various optoelectronic devices, such as green LEDs and photovoltaic cells [1, 2]. Recently, the interest in study of ZnTe thin films and its alloys has increased considerably, because of their potential application for multi-junction tandem solar cells [3]. Different techniques have been used to prepare ZnTe alloys, such as electrodeposition [4], solvothermal process [5] thermal evaporation [6], molecular beam epitaxy [7] and radio-frequency sputtering [8]. To the best of our knowledge, there are no reports so far about the synthesis of ZnTe thin films deposited by close spaced sublimation method. In the present work, we focus on the study of the influence of the substrate temperature on structural, optical properties of ZnTe and photovoltaic parameters of ZnTe/CdTe thin film solar cells based on them.

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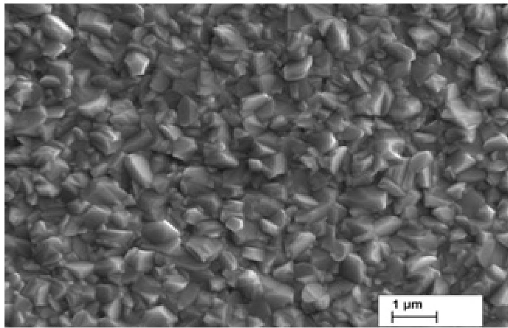
2. ZnTe DEPOSITION

The ZnTe thin films were deposited on glass substrates by close spaced sublimation method (CSS). CSS is an attractive process since it offers high depositions rates, it is able to produce films with larger grains than those deposited by other techniques and can be easily scaled up for manufacturing purposes. The 20-mm substrate–source distance of close spaced sublimation system was employed to reduce the substrate temperature. Through a series of deposition experiments at various substrate and source temperatures, it was found that for deposition of a polycrystalline ZnTe films without pinholes onto glass substrates, the substrate temperature and the source temperature should be 420°C and 590°C, respectively. A set of ZnTe thin films with different thicknesses was grown. The polycrystalline films were obtained in a short time (about 40min) without an additional transport agent gas. Forth sets of ZnTe thin films from the same source of evaporation were deposited on glass substrates. The morphology of the surface and cross section were studied using a scanning electron microscope. The structure properties of the ZnTe thin films were recorded using a Rigaku X-ray diffractometer with Cu $K_{\alpha 1}$/40kV/40mA radiation source (λ=1.54056 Å), Ni filter. The X-ray diffraction (XRD) analysis was performed using Rigaku software PDXL. The optical transmission spectra were recorded using a JASCO V-670 spectrophotometer.

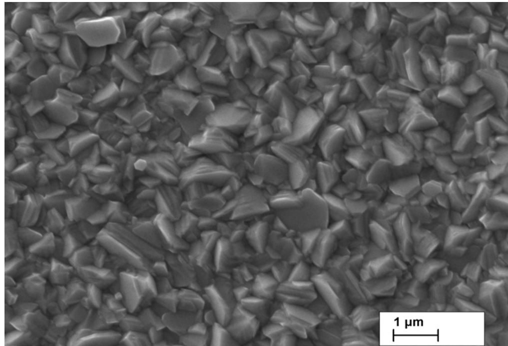
3. RESULT AND DISCUSSION

3.1. Morphology and X-ray Diffraction Studies

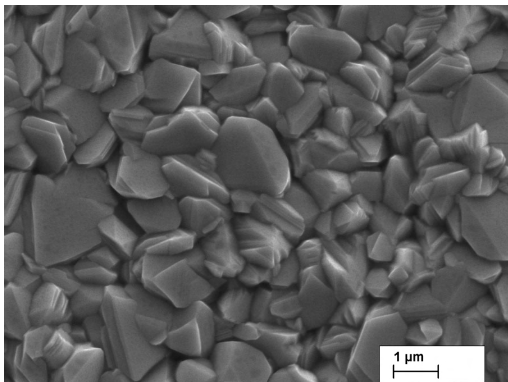
The as-deposited ZnTe thin films show uniform surface without cracks or pinholes and with good adhesion to the glass substrate.



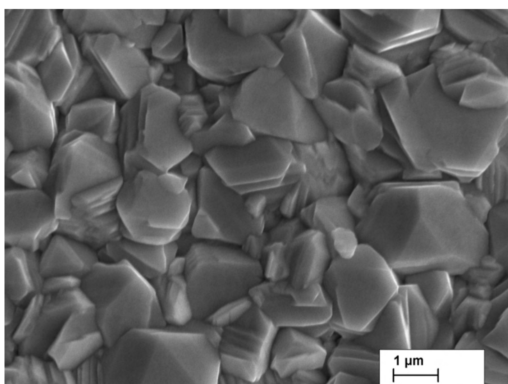
1- 0.83 μm



2 - 1.28 μm

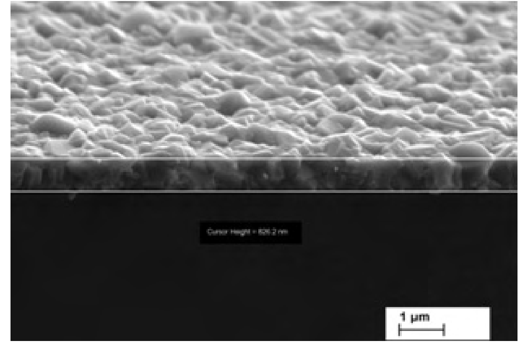


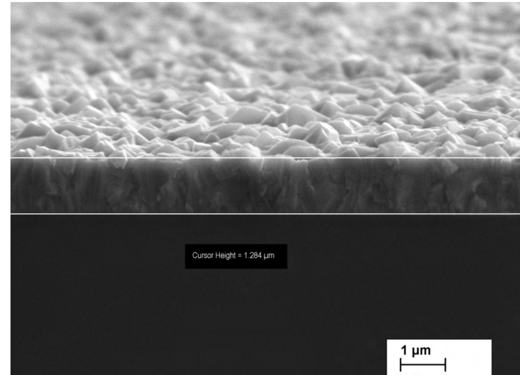
3 – 2.02 μm

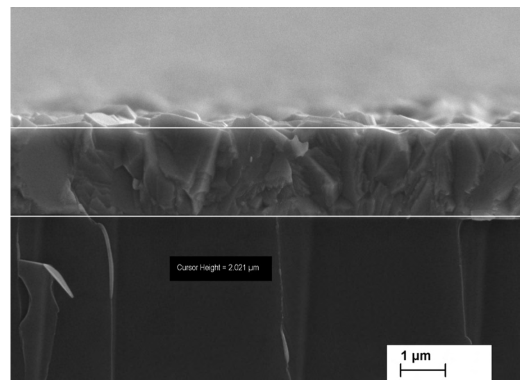


4 – 2.59 μm

Fig. 1. SEM images of the as-deposited ZnTe thin films deposited on glass substrates.







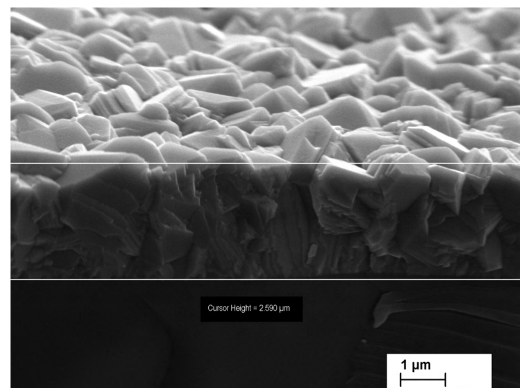


Fig . 2. Cross-section image for the same as-deposited ZnTe thin films illustrated in fig. 1.

The ZnTe thin films deposited on glass were noted as 1-4. The SEM images show that the ZnTe thin films for thicknesses < 0.5 μm have a granular structure. Fig. 1 show that with an increase of the thickness the grain sizes of crystallites increase and cross-sectional images (Fig 2) indicate that the ZnTe layer grows in a columnar morphology. The grain size of the crystallites increases from 7718 Å (0.83 μm) to 18889 Å (2.59 μm).

Analysis of XRD patterns (Fig. 3) indicates that the studied samples are polycrystalline and have a zinc blende (cubic) structure. Different diffraction peaks were identified and the corresponding values of interplanar spacing, d_{hkl} ((hkl) are Milles indices), were calculated from the Bragg equation

$$d = \frac{n\lambda}{2\sin\theta} \quad (1)$$

and compared with the standard values [6]. The lattice parameter, *a*, for ZnTe cubic phase structure was determined by the relationship

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

The sizes of the crystallites are also determined from X-ray diffraction data using the Scherrer formula

$$D = \frac{k\lambda}{\beta\cos\theta} \quad (3)$$

where *k* is the constant, *β*-is FWHM in radians, *λ*-is the wavelength of X-ray used, *θ* is the Bragg angle.

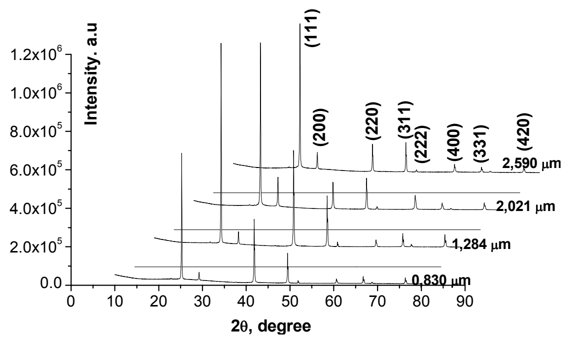


Fig. 3. The X-ray diffraction patterns of as-deposited ZnTe thin films at different thicknesses.

The XRD spectra of the ZnTe thin films exhibit the same diffraction maxima at all thicknesses, corresponding to the following crystallographic planes: (111), (200), (220), (311), (222), (400), (331), (420) and (422). The lattice parameter estimated from the position of these peaks corresponds for each sample to the value presented in the Table 1. The small change in lattice constant suggests that the film grains are a little strained in thicker ZnTe thin films, which may be owing to the charge of nature and the concentration of native defects. The ZnTe phase for all samples corresponds to the $F\bar{4}3m$ space group. Using the Williamson-Hall method, it was possible to estimate the average grain sizes of crystallites. The average size of crystallites as one can see from Table 1 increase with increasing the film thickness.

Table 1. Structural parameters of ZnTe thin films

Thickness of ZnTe layers, μm	$<D_{XRD}>$, Å	$<D_{SEM}>$, Å	*a*, Å
1 - 0,83	701,7	7718,7	6,1052
2 - 1,28	821,9	9868,8	6,1055
3 - 2,02	964,3	13077,1	6,1040
4 - 2,59	980,7	18888,8	6,1047

3.2. Optical Properties of ZnTe thin Films

In order to appreciate the optical parameters of ZnTe thin films were measured reflectance and transmission spectra at normal incidence of light on the sample surface. Energy resolution measurements don't exceed 2 meV. A transmission spectrum (Fig.4) for the sample 1 has a shape with characteristic interference maxima. Also from these curves one can see the transmittance of the layers varies between 60% - 80%, maximum of 80% being reached for ZnTe layer with lower thickness (0.83 μm). With increasing the thickness (from 0.83 μm to 2.59 μm) the spectra show a decrease of transmission near the fundamental absorption,

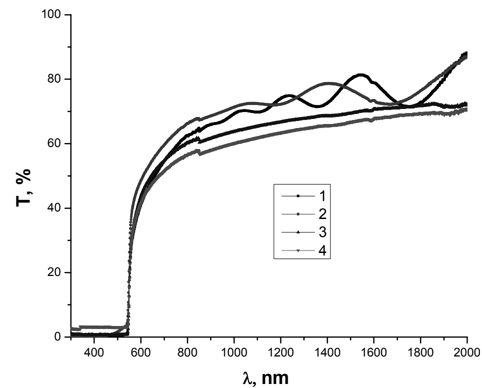


Fig. 4. Transmission spectra of as-deposited ZnTe thin films.

which is identifying a good crystallinity of obtained layers. The absorption coefficient, α, was calculated from expression

$$\alpha = \frac{1}{d} \ln \frac{(1-R)^2}{T} \quad (4)$$

where d is the film thickness, and R and T represent the reflection and transmission coefficient, respectively. The absorption coefficient dependencies are presented in Fig.5. By taking into account optical band-to-band transitions ZnTe are considered to be direct semiconductors [2].

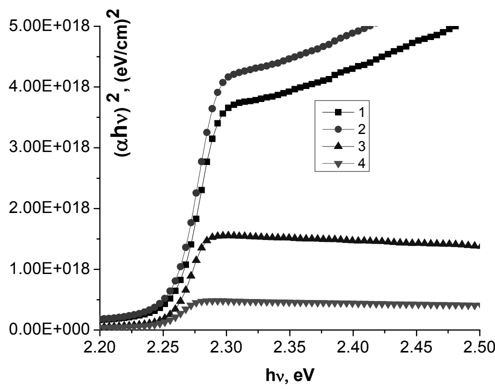


Fig. 5. Dependence of $((\alpha h\nu)^2$ as a function of the photon energy (hν).

Therefore, the energy dependence of absorption coefficient, α, near the fundamental absorption band edge for band-to-band transitions is described by expression

$$\alpha h\nu = A_\alpha (h\nu - E_g)^{1/2} \quad (5)$$

where $h\nu$ is incident photon energy, a A_α denotes a characteristic parameter (independent of photon energy) for respective transitions, and E_g is energy bandgap. The optical energy gap, E_g, was determined by extrapolating the linear portions of $(\alpha h\nu)^2 = f(h\nu)$ dependences to $(\alpha h\nu)^2 = 0$. For studied samples the optical bandgap values ranged between 2.259 eV (0.83 μm) and 2.256 eV (2.59 μm).

4. CONCLUSIONS

The XRD reveals that the as-grown ZnTe layers were polycrystalline presenting cubic structure. When thickness increases the average grain size increases. The variations in lattice constants for the thicker deposited ZnTe films over the bulk values suggest that film grains are strained. The optical absorption study shows a smaller variation of band gap of ZnTe thin films. The optical transition is found to be direct and allowed.

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