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Study of structure and optical properties of CdSe thin films

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This paper reports optical properties study of thermal vapour deposited CdSe thin films on glass substrate. The films thickness of 0.21-1.24 μm was measured using an interferometric method. The CdSe thin film was investigated with TEM, SAED, XRD, and AFM techniques. A hexagonal structure was revealed for all investigated samples. The optical absorption spectra obtained were in the 400-1400 nm range. The maximum and minimum in the spectra are due to the multiple reflexion on the surfaces of the film, indicating that the samples were uniform. The refraction index and the band gap Eg of CdSe films were determined from the absorption spectra.

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1. Introduction

Metal chalcogenides (sulfides, tellurides and selenides) are of great importance for nowadays energy issues because they are potential candidates for optoelectronic applications such as photodetectors, solar cells, thin film transistors etc. Cadmium selenide (CdSe) thin films are among the most commonly used window materials for high efficient cadmium telluride (CdTe) and chalcopyrite polycrystalline thin-film photovoltaic devices. For the development of such optoelectronic devices, CdSe thin films require comprehensive optical characterization [1-5].

However, usually different structures appear, with different grain sizes and energy gaps in CdSe polycrystalline films, which imply that the influence of growth process on the structures and properties of CdSe thin films must be considered. The substrate, thickness, composition, crystalline structure and grain size of the films strongly influence the optical properties.

In the present work, we report a study on the optical properties of such CdSe thin films as the knowledge about their parameters is very important in many scientific, technological and industrial applications in the field of optoelectronic devices, particularly solar cells.

2. Experimental

High purity (99.999 %) CdSe powder was used in the material preparation. CdSe films varying in thicknesses between 0.21-1.24 μm were prepared by the limited volume thermal evaporation technique under vacuum, using an semiautomatic VUP-5 device and the following parameters [6,7]: support temperature during the deposition T_s=290-550K, evaporator's temperature T_{ev}=110-1200K, evaporator-substrate distance D=9cm, deposition rate r_d=5.4-12 Å/s. The deposit thickness was measured with interferential microscope [8]. The thin film structure and its superficial morphology were studied with XRD (X-ray diffraction) method, AFM (Atomic Force Microscopy), TEM (Transmission Electronic Microscopy), ED (Electronic Diffraction) methods. The films showed a predominant hexagonal phase with small crystallites. The optical band gap of the films was estimated using the optical transmittance measurements. The optical transmission and absorption spectra were obtained within the range of 300-1400nm. From the absorbance data, the absorption coefficient α was calculated. Using the absorbance data the optical band gap and refraction index n were determined [9-13].

3. Results and discussion

CdSe thin films structure was studied using XRD (Fig.1) in the angular range 20-70° with the CoK_α radiation. All studied samples are polycrystalline and have a wurtzite (hexagonal) structure. The crystallites are highly oriented with the (002) planes parallel to the substrate [14,15,16].

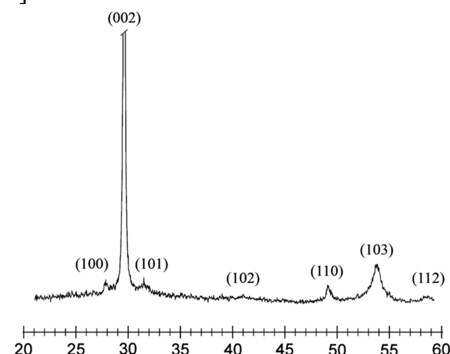

Fig. 1. XRD pattern (CoK_α radiation) for a CdSe film (T_{ev} = 980 K, T_s = 400 K, d = 1,24 μm).

The CdSe thin films surfaces were analyzed with AFM and a grain-like compact layer surface morphology was revealed. Generally, the roughness of the film surfaces was found small with an average roughness of several nanometers (Fig. 2).

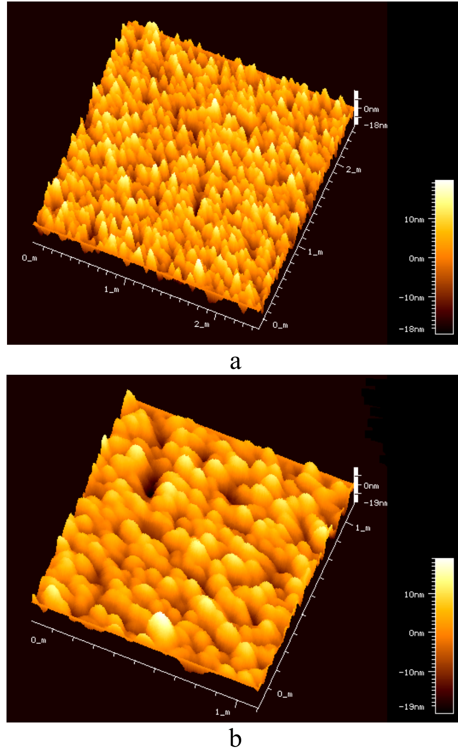

Fig. 2. AFM image for 1.24μm thickness sample 3μm x 3μm (A), AFM image for 1.24μm thickness sample 1μm x 1μm (B).

A SAED image with the indexed difraction rings (Fig. 3) was obtained on the CdSe poycristaline thin film. The dark zones show a begining of prefferential orientation, the (002) planes being much more intense in those directions. The indexing correspond to hexagonal CdSe of spatial group P63mc and reticular parameters a = 0.42990 nm and c = 0.60100 nm.

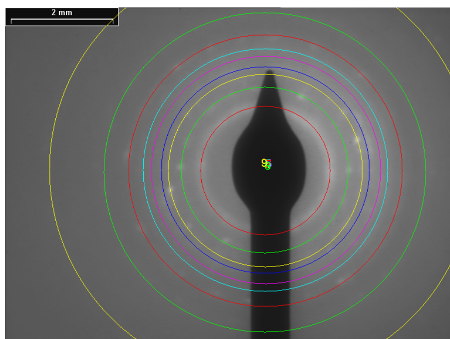

Fig. 3. Electron diffraction pattern for CdSe film 1.24 μm thick

Transmission coefficient strongly depends on film structure, determined by the film thickness and deposition conditions. A sharp absorption edge at a wavelength corresponding to bandgap energy indicates a stoichiometric composition (Fig. 4).

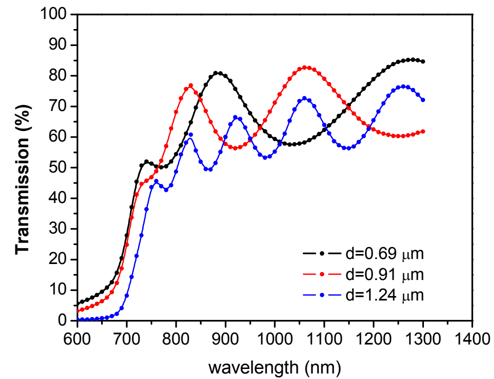

Fig. 4. Transmission spectra for investigated CdSe films

The refraction index, in the spectral domain of medium and strong transmission, is calculated using the Swanpoel's method [13] of creating envelopes of the interference maxima and minima (Fig. 5).

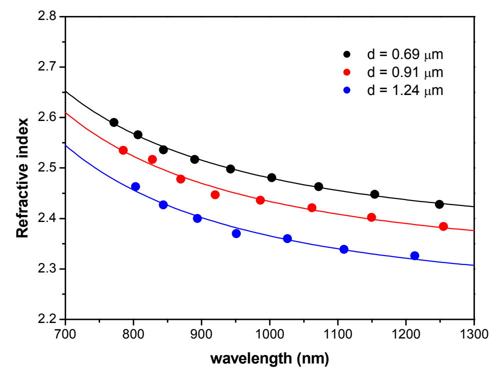

Fig. 5 Refraction index for CdSe thin films

The dependences $(\alpha h\nu)^2=f(h\nu)$ for studied sample and confirms the direct nature of band-to-band transitions. The values of bandgap ranged between 1.69 eV and 1.75 eV [17-19].

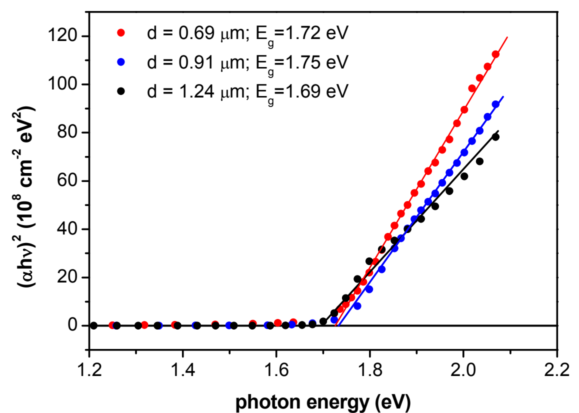

Fig. 6. $(\alpha h\nu^2)$ vs. photon energy dependency for the studied samples.

4. Conclusions

CdSe thin films are polycrystalline and exhibit a wurtzite structure. The values of the optical bandgap energy, calculated from the absorption spectra, ranged between 1.69 eV and 1.75 eV. For the studied samples, the $(\alpha h\nu^2)$ vs. photon energy dependency is linear, which shows direct optical transitions, according with the elsewhere studied results on the energetic band structure of this material.

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