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Preparation and structural characterization of thin-film CdTe/CdS heterojunctions

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The structural characteristics of CdTe/CdS thin-film heterojunctions are investigated. The studied heterojunctions were obtained by successive thermal evaporation under vacuum onto unheated SnO_2 coated glass substrates of CdS and CdTe films, respectively. The morphological and structural studies of the above mentioned heterojunction component films, in comparison with those of CdS and CdTe films, deposited separately, onto glass substrates, were carried out using transmission electron microscopy, X-ray diffraction and atomic force microscopy techniques.

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Keywords: CdTe, CdS, Thin films, Heterojunctions, Structural properties

1. Introduction

CdTe/CdS heterostructures are intensively studied due to their important applications in the technology of high efficiency thin film solar cells. Usually, the solar cells based on CdTe/CdS heterojunction are prepared in multilayered configuration by subsequently deposition onto transparent conducting oxide (TCO) coated soda-lime glass substrates of n-CdS, p-type CdTe films and a metallic back contact [1-5]. The efficiency of such solar cells is strongly influenced by the structure and the physical properties of component films. For this reason, most of the research efforts have been concentrated on the study of preparation conditions – properties relationship for individual CdS and CdTe layers [6], deposited onto different substrates, mainly on glass substrates. But in the respective solar cells, both the CdTe and CdS films are deposited onto the certain substrate: CdS onto TCO and CdTe onto CdS substrates, respectively. This fact may influence the structure of respective layers and consequently their physical properties.

In present paper, the structural characteristics of the CdS and CdTe films, component of In/CdTe/CdS/SnO_2/glass heterostructure, in comparison with those of CdS and CdTe films deposited in the same conditions onto glass substrates, are investigated.

The morphological and structural characterization of the above mentioned films were performed by atomic force microscopy (AFM), transmission electron microscopy (TEM) and X-ray diffraction (XRD) techniques.

2. Experimental

The studied samples were prepared as follows. First, metallic Sn was evaporated in vacuum onto clean glass substrates with 2×2 cm^2 area, maintained at temperature of 350 K. The Sn source temperature was 1450 K. In order to obtain transparent conductive SnO_2 films, the Sn coated glass substrates were then heat treated in air, for thermal oxidation, for 30 min in the 300 K – 700 K temperature range, using isochronial annealing. The CdTe/CdS heterojunctions (HJ) were grown on these transparent SnO_2/glass substrates by successive depositions under vacuum ($p \approx 10^{-5}$ Torr) by quasi-closed volume technique [7], of CdS (of thickness d = 0.42 μm) and CdTe (d = 1.32 μm) films. The temperatures of resistively heated tungsten crucibles for CdS and CdTe polycrystalline powders were 1200 K and 870 K respectively. Finally, the indium electrode was evaporated in vacuum onto CdTe/CdS/SnO_2/glass system.

To permit AFM surface analysis of both CdTe and CdS HJ component layers, they were deposited with different diameters, using special masks. In Fig. 1 the top and cross views of as obtained multilayers are shown.

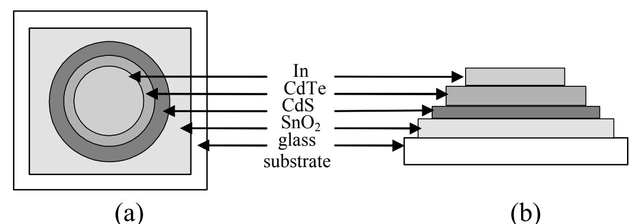


Fig. 1. Schematic drawing of the obtained multilayered system: (a) top view, (b) cross-section.

To investigate the influence of substrate nature on the structural characteristics of CdTe/CdS heterojunctions, simultaneously with these, CdTe and CdS reference thin films were deposited separately, onto glass substrates, under the same conditions as the respective HJ component films. The distance evaporator-substrates were for all depositions of 8 cm.

Other details of the experimental procedures weregiven elsewhere [8].

The structure of studied samples was investigated using XRD technique, with CoKα radiation (λ = 0.1790 nm) in the range of 2θ = 20° – 60°.

Atomic Force Microscope (AFM) in the tapping mode was used to study the surface topography of CdS and CdTe films. A commercial standard silicon cantilever NSC

21 having a force constant of 17.5 N m^{-1}, 210 kHz resonance frequency and tip with radius of 10 nm was used.

The structural characteristics of HJ were also studied by TEM technique.

3. Results and discussion

In Figs. 2 and 3 are shown the typical 3µ × 3µ AFM micrographs of CdS and CdTe films, deposited both onto glass substrates and as HJ components, respectively. The values of average R_a, and root mean square, R_{rms}, surface roughness for respective samples are given in Table 1. Also, the typical grain height distributions for respective samples are shown in Fig. 4.

From respective figures, one can observe that the nature and morphology of film substrates influence the surface morphology both for CdS and CdTe films. In the case of CdS and CdTe films deposited onto glass substrates, the column-peaks are more closely packed and the surface roughnesses are smaller in comparison with those for CdS and CdTe HJ component films. Also, the deposition of last films onto the substrates of other chemical nature (SnO_2/glass for CdS film and CdS/SnO_2/glass for CdTe film, respectively) determines an increase of the film crystallite size. As it results from Fig. 2a, the crystallite size of CdS film deposited onto glass substrate ranged between 0.1 µm and 0.2 µm, whereas, those for HJ CdS component film varied in 0.2 µm – 0.3 µm range (Fig. 2c). The similar conclusion results from Fig. 3a,c for CdTe films. For such films, the crystallites size varied in the 0.05 µm – 0.1 µm range for CdTe film deposited onto glass substrates and in 0.2 µm – 0.3 µm range for HJ component CdTe film.

The roughness of surface substrate also influences the surface morphology and grain height distribution for respective samples.

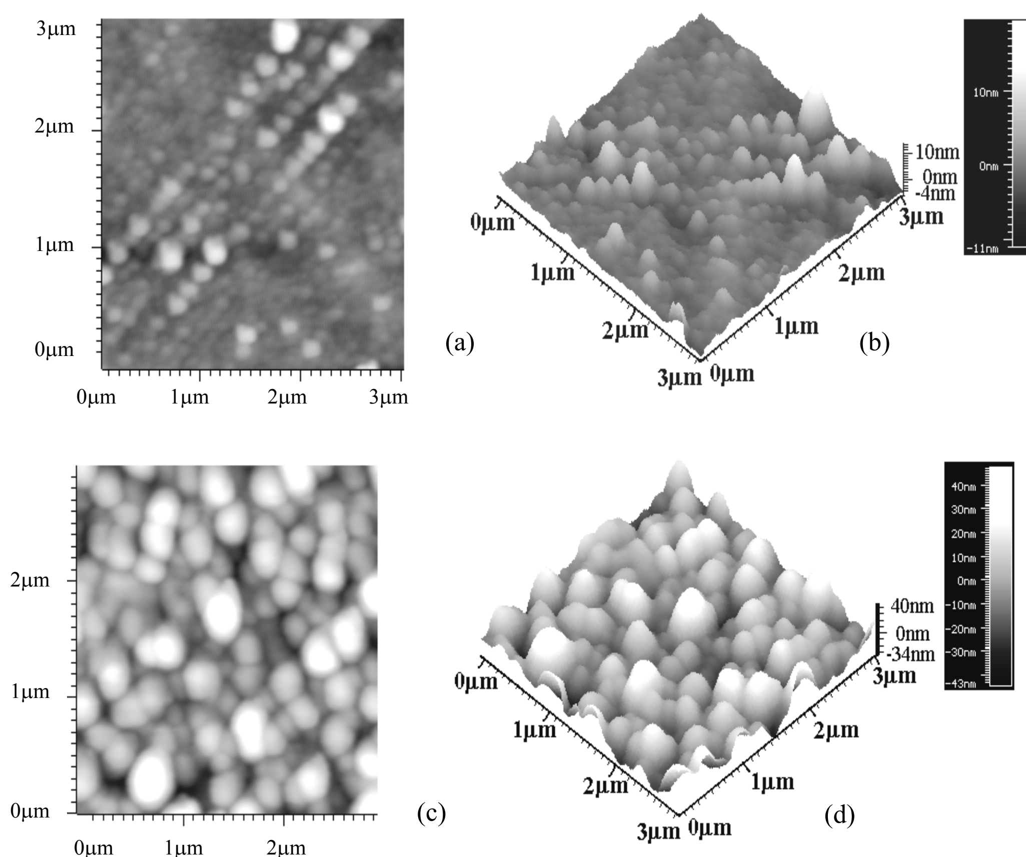


Fig. 2. Two (a,c) and three (b,d) dimensional AFM images of the surface of CdS films: (a,b) – deposited onto glass substrate; (c,d) – component of HJ.

Table 1. Roughness parameters of CdS and CdTe films.

film/substrate	R_a (nm)	R_{rms} (nm)
CdS/glass	1.4	2.0
CdS/SnO_2 (HJ)	10.3	12.9
CdTe/glass	0.5	0.7
CdTe/CdS (HJ)	8.9	11.3

As it results from Table 1, the values of R_{rms} of the CdS films deposited onto glass substrate and onto SnO_2/glass substrate is 2.0 nm and 12.9 nm respectively, hence the HJ component CdS films have about of six times as rough surface. A greater R_{rms} has the CdTe film from HJ, comparative with similar CdTe film deposited onto glass substrate.

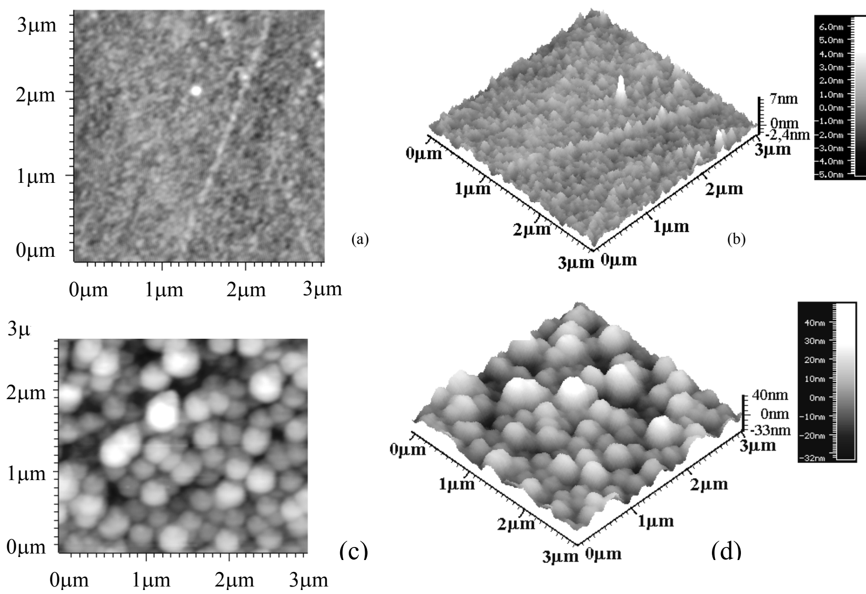


Fig. 3. Two (a,c) and three (b,d) dimensional AFM images of the surface of CdTe films: (a,b) – deposited onto glass substrate; (c,d) – component of HJ.

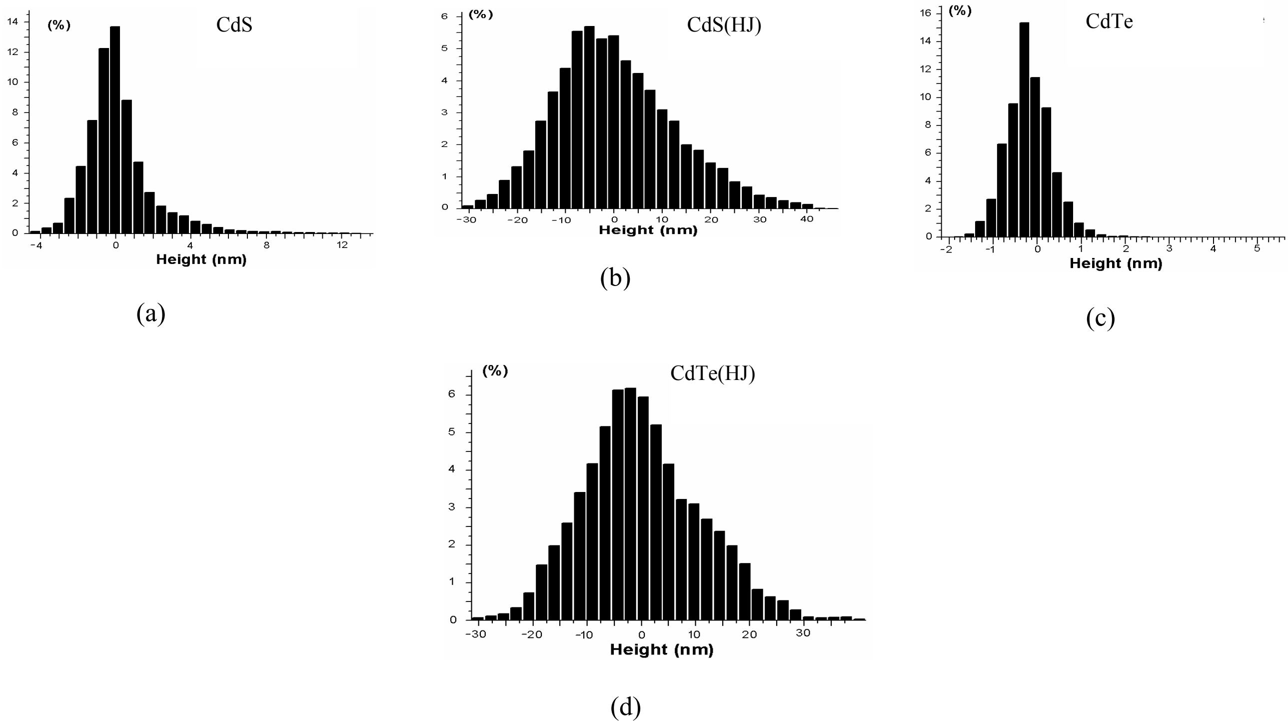


Fig. 4. Grain height distributions of CdS (a,b) and CdTe (c,d) films: (a,c) deposited onto glass substrate; (b,d)-component of HJ.

From Fig. 4, also results that both CdTe and CdS films, component of HJ, are characterized by a greater dispersion of grain height.

The rougher surfaces of HJ component films can be attributed to the rough surface of their substrates (SnO_2 for CdS and CdS for CdTe films, respectively). This can determines the grown and coalescence of randomly oriented grains of different sizes. Although the CdTe and CdS HJ component films are deposited onto different substrates, the similar results regarding the increase of their surface roughness are obtained. This indicates that, in the case of HJ component films, the surface roughness of film substrate plays a greater role in the film surface morphology than the chemical nature of respective substrate.

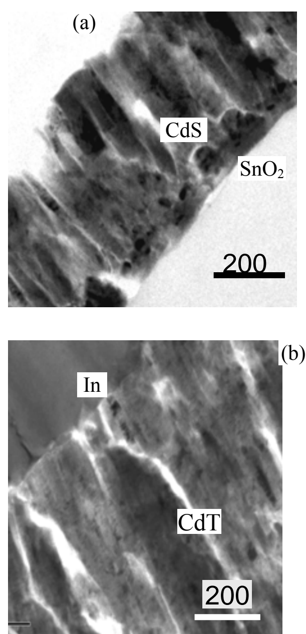


Fig. 5. The BF/TEM cross-section micrographs of (a) CdS and (b) CdTe films components of In/CdTe/CdS/SnO_2/glass system. The SnO_2 and In layers of this system are also shown.

In Fig. 5, the TEM dark-field cross-sections micrographs of CdS and CdTe films, component of In/CdTe/CdS/ SnO_2/glass system can be seen. A structure of columnar crystallites both for CdS and CdTe films can be observed. Also, a well-defined interface between CdTe and In layer can be seen in Fig. 5b, whereas, those between CdS and SnO_2 films is more rough (Fig. 5a). This last fact can explain the rougher surface of CdS films deposited onto SnO_2/glass substrate, revealed by AFM image from Fig. 2d.

Electron microscopic studies were also made on the HJ component CdS and CdTe films. In Fig. 6a,b, the typical selected electron diffraction (SAED) patterns for CdS and CdTe films, component of HJ, are presented.

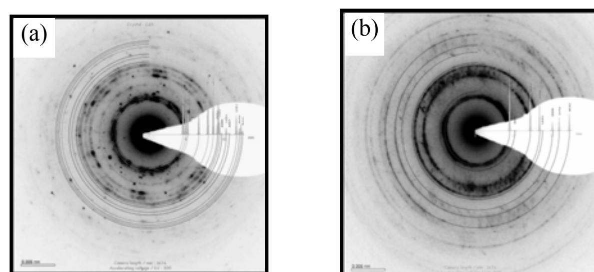


Fig. 6. SAED patterns for the same films as in Fig. 5 (a) CdS film, (b) CdTe film. (Inset shown the corresponding diffraction peaks).

The electron diffraction rings corresponding to the reflection from various set of planes indicate a polycrystalline structure both for CdS and CdTe films. The indicated peaks in Fig. 6 are in good agreement with ASTM cards for CdS [9] and CdTe [10], respectively, and reveal a hexagonal wurtzite structure for CdS film and a cubic sphalerite structure for CdTe film. The presence of all main diffraction peaks in respective patterns indicates that both CdS and CdTe films present a lower preferred orientation of their crystallites.

Unlike HJ component CdS and CdTe films, those deposited onto glass substrates, present a textured structures. In Fig. 7a,b, the X-ray diffraction patterns for CdS and CdTe films, deposited onto glass substrates, simultaneously with those from Fig. 6, are shown.

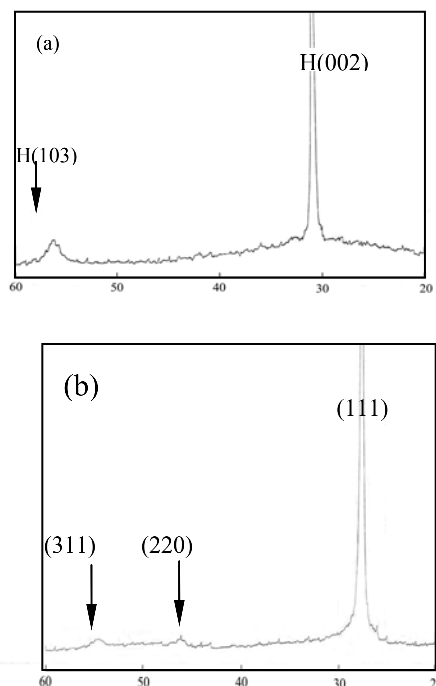


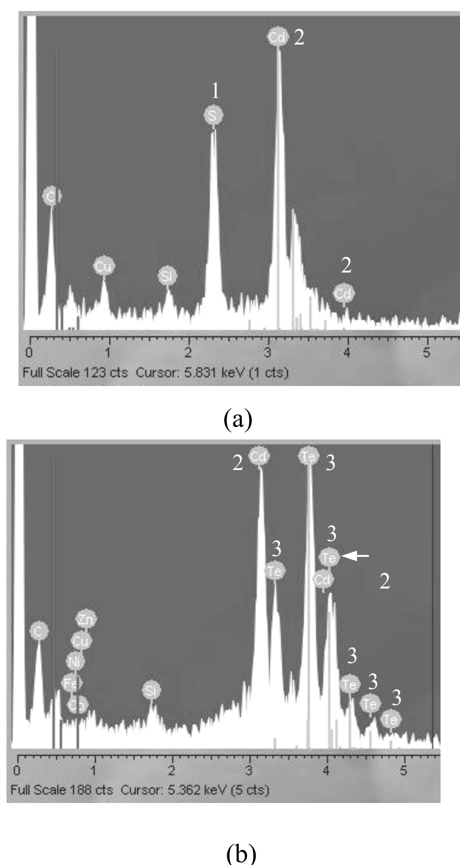
Fig. 7. Typical XRD patterns (CoKα radiation) of (a) CdS and (b) CdTe films, deposited onto glass substrates simultaneously with those from Fig. 6.

As it results from Fig. 7a, the diffraction pattern for CdS film contains one prominent peak, at $2\theta = 31.06°$, corresponding to (002) set planes and other shallow peak at $2\theta = 56.5°$, of low intensity, corresponding to reflection on (103) planes. This indicates a hexagonal wurtzite structure of the film and preferential growth of crystallites with (002) planes parallel to the substrate, hence with c-axis perpendicular to the substrate.

A textured structure also present the CdTe films deposited onto glass substrates. The intensity peak at $2\theta = 27.7°$ from Fig. 7b indicates the cubic <111> texture of respective film. The relative intensities $I_{002}/I_{103} = 16.2$ characteristic for respective CdS film and $I_{111}/I_{220} = 39.5$ for CdTe film, grater respectively than 0.62 [9] and 1.66 [10] for standard powder samples confirm above observations. Such orientation grown of the crystallites both in CdS and CdTe films deposited onto glass substrates at lower temperature have been revealed by other researches [11-13], and have been attributed to the lower interfacial energy of the film and glass substrates, compared with the higher atomic plane density in the film surface adjacent to the substrate [11,14]. In the case of CdS and CdTe films which compose the respective HJ, both of them have been grown on the other and rough substrates (CdS onto SnO_2 and CdTe onto CdS,

respectively). This fact can affect the mobility of evaporated atoms on the respective substrates and hence to led to a randomly oriented crystallite grown, as it results from SAED patterns from Fig. 6. This conclusion is in good agreement with the above AFM results related to the modification of crystallite grown mode when the film substrate is changed.

Energy dispersive X-ray analysis (EDAX) was carried out to investigate the composition of HJ component films (Fig. 8).



(b)

Fig. 8. EDAX spectra of HJ component films: (a) CdS film, (b) CdTe film. (1 – S; 2 – Cd; 3 – Te; The non specified peaks belong to the sample holder and not to the thin film itself).

The obtained results regarding the CdTe and CdS component films revealed a Te enriched composition with about 4 at% for CdTe layer and about 2 at% sulf deficiency in CdS layer. Such deviations from stoichiometry are also characteristic both for CdTe and CdS films evaporated onto unheated glass substrates [8,15,16].

4. Conclusions

Thin film CdTe/CdS heterojunctions were prepared by thermal evaporation in vacuum in the In/CdTe/CdS/SnO_2/glass multilayerd system. By AFM, TEM and XRD measurements, the structural characteristics of HJ component CdTe and CdS films, in comparison with those of CdTe and CdS films, separately deposited onto glass substrates, were investigated. The obtained data revealed that the CdS and CdTe films deposited onto glass substrates present a polycrystalline c-axis and <111> textured structures, respectively, and lower surface morphologies. Unlike of these, those from HJ present a columnar polycrystalline structure without preferred orientation. Also, their surface roughnesses are more than six times greater than those of CdTe and CdS films deposited onto glass substrates.

These results indicate that the chemical nature and especially surface morphology of the film substrates influence both the texture and surface morphology of CdS and CdTe films, component of studied heterojunctions.

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