

Effects of proton irradiation on CdTe thin films used in photovoltaic applications

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The effects of irradiation with high energy protons (3 MeV), at 3×10^{14} fluency, on structural and optical properties of polycrystalline CdTe thin films used in photovoltaic applications have been investigated. XRD investigation has revealed that the films contain a cubic phase of CdTe, preferentially oriented along $<111>$ direction. The irradiation only produced slight modifications on the XRD pattern. A slight decrease of the optical bandgap of the samples was observed after irradiation.

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1. Introduction

CdX (X – chalcogen) compounds are interesting for solar cells based on thin film technology applications because of their suitable bandgaps, large absorption coefficients and good chemical stability. Moreover, they can be manufactured using low-cost techniques. Because of its unique properties, CdTe is an ideal material for applications such as photovoltaic cells [1-4] or nuclear detectors [5].

For instance, CdS/CdTe heterostructures have been extensively studied [1-3] in the last few years, a good photovoltaic conversion efficiency being obtained for such structures.

The performance of the devices based on thin film technology strongly depends on the physical properties of the films. Therefore, it is important to identify the defects having influence on electrical and optical properties of the films. Electrical properties of the CdTe thin films were investigated by many researchers [6-10], but studies on the influence of the ionizing radiations on their properties are still very scarce.

In this paper we report the changes induced by irradiation with high energy protons (3 MeV, fluencies of 3×10^{14} protons/cm²) on the structural and optical properties of CdTe thin films, using XRD and optical measurements. Such a study is justified by the prospective use of CdTe thin films for producing solar cells for space technology applications.

2. Experimental results and discussion

CdTe thin films were deposited by thermal vacuum evaporation from a single source on glass substrates. CdTe powder (Aldrich) was vacuum sublimated from a quartz evaporator heated to 750 °C. The evaporator was covered

with a quartz-wool plug, to prevent the sputtering of the powder during deposition. The residual pressure in the evaporation chamber was below 10^{-5} Torr. The substrate temperature was maintained at 270 °C during deposition. Finally, to improve the structural and chemical homogeneity of the films, they were thermally treated in vacuum at 350 °C for 15 min.

The samples were irradiated in vacuum with protons supplied by an accelerator. The incident proton beam was directed perpendicularly to the surface of the samples. Irradiation was performed in an evacuated chamber, at ambient temperature, with protons of 3 MeV energy at 3×10^{14} protons/cm² fluency. The thermal effect during irradiation was negligible.

The crystallinity of CdTe films was characterized by X-ray diffraction (XRD), using a high resolution X-ray diffractometer (D8 Discover – Bruker). XRD spectra were recorded by using CuK_{α1} line, $\lambda = 1.5406$ Å, with a detector-scan method and a stationary incident beam at grazing incidence, for reducing the diffracted intensity from the substrate. The scanning step was $\Delta(2\theta) = 0.05$ Å.

Optical measurements were performed before and after irradiation, for identifying the defects induced by high-energy protons irradiations. Optical absorption and absolute reflection spectra were measured by using a Perkin Elmer Lambda 35 UV/VIS spectrophotometer, equipped with an integrating sphere. The absolute reflectance was measured at an incident angle of 8°.

Structural analysis of the samples by X-ray diffraction revealed that the CdTe films contain a cubic, zincblende type phase. The films exhibit a polycrystalline nature, containing crystallites with different orientations perpendicular to substrate surface, with most of crystallites oriented with (111) planes parallel to the substrate. XRD patterns are shown in figure 1 and data regarding crystallite sizes D_{eff} are collected in table I.

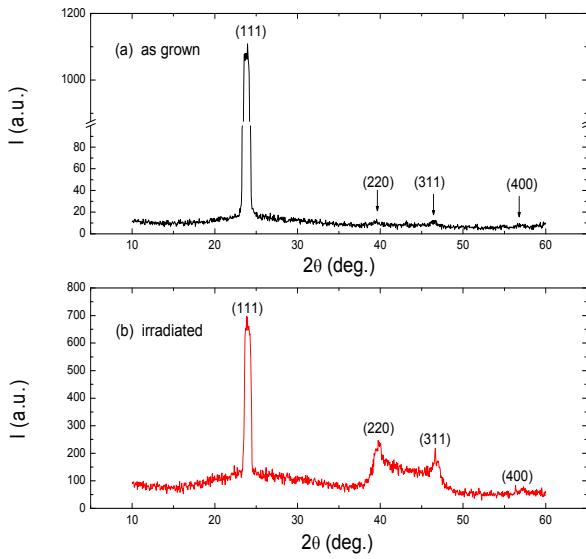


Fig. 1. Experimental X-ray diffraction pattern of CdTe films (a) as grown and (b) irradiated.

Table 1. Crystallite sizes of CdTe films, determined by using equation (1).

Sample	D _{<111>} (Å)	D _{<220>} (Å)	D _{<311>} (Å)
as grown	100	95	131
irradiated	100	93	133

Crystallite sizes were determined using Scherer's formula:

$$D_{\text{eff}} = \frac{0.9 \lambda_X}{\delta \cos \theta_0} \quad (1)$$

where λ_X is the x-ray wavelength, δ is the full width at half maximum of the corresponding peak and θ_0 is the angle where the peak occurs. There is no change in the position of the observed peaks after irradiation, but the intensity of (111) peak decrease, while the intensity of (220) and (311) peaks increase.

Fig. 2 shows near-threshold absorption spectra, before and after irradiation, for one of the analyzed samples.

The optical bandgap of the films was determined by using the well known equation, valid in the case of allowed direct transitions in semiconductors:

$$\alpha = \alpha_0 \frac{(h\nu - E_g)^{1/2}}{h\nu}, \quad (2)$$

where α is the absorption coefficient, $h\nu$ is the energy of incident photons, E_g is the bandgap, and α_0 is a quantity not depending on photon energy.

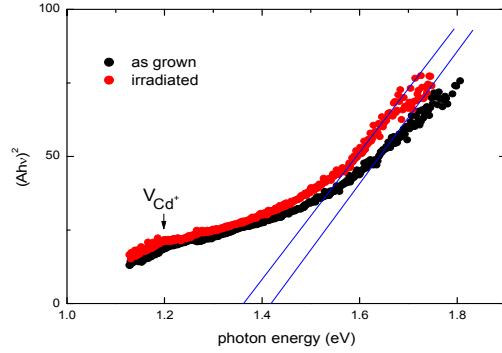


Fig. 2 $(A \cdot h\nu)^{1/2}$ versus $h\nu$ dependence of as grown (a), and irradiated (b) CdTe films, measured at 295 K.

A value of 1.42 eV was determined for the bandgap in the case of the as grown sample. The bandgap decreased to 1.38 eV after irradiation.

Also, one can observe a shoulder in the absorption spectra, below the threshold, at about 1.2 eV, its magnitude increasing after the irradiation. It was argued (see, for example, Ref. 11) that the defect state with an energy level located at 0.2 eV above the valence band in CdTe corresponds to simply ionized Cd vacancies. Therefore, the observed feature can be tentatively associated to Cd vacancies. This is also supported by the fact that its magnitude increases after irradiation, Cd vacancies being largely produced by proton irradiation.

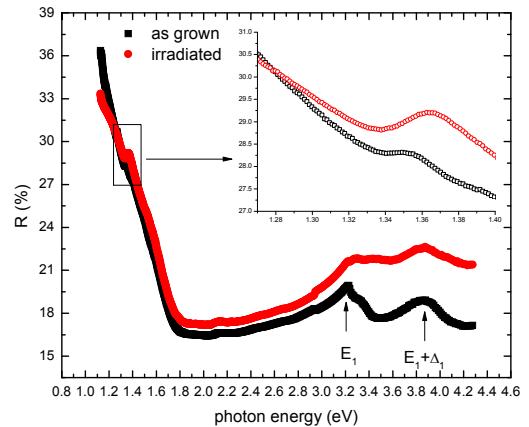


Fig. 3. Reflection spectra measured at 295 K, before (squares) and after (circles) irradiation.

Fig. 3 shows the reflectance spectra, measured before and after irradiation. One can observe an increase of the total reflectance after irradiation, in the high energy part of the spectrum. This is probably related to a surface reconstruction during the exposure to the proton beam. The extrema E_1 (at critical point energy 3.24 eV) and $E_1 + \Delta_1$ (at critical point energy 3.88 eV) are very close to

the values recorded for bulk samples, respectively 3.28 eV and 3.88 eV [12]. After irradiation those two extrema got less pronounced. This correlates to the observed increase of structural disorder (see XRD data presented above).

3. Conclusions

An investigation on the effects of high energy proton irradiation on structural and optical properties of CdTe films grown by vacuum deposition was performed. XRD investigation revealed that the films contain a cubic zincblende type phase, with most of the crystallites having $<111>$ planes parallel to the substrate. The fundamental absorption edge before irradiation is found to be 1.42 eV (at 295 K), value which after irradiation decreased down to 1.38 eV. A shoulder, more pronounced after irradiation, was observed in the absorption spectra, at 1.2 eV photon energy. It was tentatively associated to simply ionized Cd vacancies. Reflection spectra were measured before and after irradiation, at 295 K. The most important changes can be seen in the high energy region of those spectra, where the extrema at critical point energies E_I and $E_I + \Delta_I$ got less pronounced after irradiation, while the reflectance increased.

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