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## Structural and optical properties of $\text{Cd}_{1-x}\text{Zn}_x\text{Te}$ thin films

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Received 29 June 1994; in final form 26 July 1994

### Abstract

Polycrystalline thin films of  $\text{Cd}_{1-x}\text{Zn}_x\text{Te}$  ( $x=0.0$  to  $0.5$ ) deposited by co-evaporation of CdTe and ZnTe in a vacuum better than  $5 \times 10^{-6}$  Torr on Corning 7059 glass substrates maintained at  $300^\circ\text{C}$  and subsequently annealed in vacuum at  $400^\circ\text{C}$  for 1 h were found to be single-phase and nearly stoichiometric. The structural, electrical and optical properties of these films were studied. The lattice parameter and the optical energy gap in relation to the composition were estimated and the results are discussed in detail.

**Keywords:** Co-evaporation; Structural properties; Optical properties; Thin films

### 1. Introduction

In recent years II–VI compound semiconductors have become very popular because of their potential application for bandgap engineering. Among these, CdTe is one of the best suited materials for photovoltaic solar energy conversion, owing to its optimum direct bandgap ( $E_g = 1.5$  eV). Several investigators have fabricated CdS/CdTe solar cells and obtained efficiencies in excess of 10% [1–3]. Although the maximum theoretical efficiency of the n-CdS/p-CdTe heterojunction is 19.7% under air mass zero (AM0) condition, the actual cell performance was limited by problems concerning the conductivity control of, and the realization of low resistance ohmic contact on, p-type CdTe [4]. Meyers [5] proposed a novel n–i–p solar cell structure of the type p-ZnTe/i-CdTe/n-CdS in which CdTe was used as an intrinsic absorber layer, thereby avoiding the above-mentioned problems, and obtained an efficiency of 11.2%. Recently Simmons [6] fabricated monocrystalline p-ZnTe/i-CdTe/n-CdS solar cells by sequential metalorganic vapour phase epitaxy of ZnTe and CdTe layers on CdS substrates and obtained cell efficiencies up to 13% under air mass one (AM1) illumination. This led to new interest in the development of wide bandgap absorbers based on the alloys of ZnTe and CdTe with a variety of advantageous properties. The bandgap and lattice parameters of  $\text{Cd}_{1-x}\text{Zn}_x\text{Te}$  films can be tuned to desired values by controlling the composition of the films.  $\text{Cd}_{0.7}\text{Zn}_{0.3}\text{Te}$  films with a bandgap of about 1.7 eV can advantageously be used

as a top cell absorber material in tandem solar cells. A 10% efficient top cell based on  $\text{Cd}_{1-x}\text{Zn}_x\text{Te}$  with energy gap 1.7 eV and about 80% sub-gap transmission coupled with a 12–15% CuInSe<sub>2</sub>-based bottom cell configuration can produce a combined cell efficiency of 15–20% [7].

Thin films of  $\text{Cd}_{1-x}\text{Zn}_x\text{Te}$  were prepared by a variety of techniques, such as two-source vacuum evaporation in coaxial tubes [8], molecular beam epitaxy [9], chemical vapour deposition [10], metalorganic chemical vapour deposition [11] and two-stage process [12]. All these methods of film preparation have their inherent advantages and disadvantages. This paper describes the growth of single-phase polycrystalline  $\text{Cd}_{1-x}\text{Zn}_x\text{Te}$  films ( $x=0.0$  to  $0.5$ ) by a two-source vacuum evaporation technique. The structural, electrical and optical properties of these films were studied in relation to the composition ( $x$ ) of the films.

### 2. Experimental

In the present investigation the two-source vacuum evaporation method or the three-temperature technique, also known as the Gunther technique [13], was employed to prepare thin films of  $\text{Cd}_{1-x}\text{Zn}_x\text{Te}$ . This technique has the advantage of better control over deposition parameters. The two sources are positioned apart such that the substrates are exposed uniformly to both the vapour streams. A specially designed screen was placed exactly in-between the two sources to isolate

individual vapours at the beginning. The thickness and the rate of evaporation were monitored by a quartz crystal thickness monitor. The individual rates of deposition of the two sources were calibrated in terms of the source current and the source temperature using a temperature controller. To deposit films of the required composition, sufficient quantities of 5N pure CdTe and ZnTe (obtained from M/S Balzers, Switzerland) were taken into the two separate crucibles. The system was evacuated to a vacuum better than  $5 \times 10^{-6}$  Torr. The glass substrates (Corning 7059) were maintained at a temperature of 300 °C. Keeping the deposition rate of CdTe constant at  $20 \text{ \AA s}^{-1}$ , the rate of deposition of ZnTe was varied to obtain films of different compositions. To homogenize the films they were subsequently annealed in vacuum at 400 °C for 1 h.  $\text{Cd}_{1-x}\text{Zn}_x\text{Te}$  films with  $x$  in the range 0.0–0.5 were grown in the present studies.

X-ray diffraction (XRD) spectra of the  $\text{Cd}_{1-x}\text{Zn}_x\text{Te}$  films were obtained using a Philips X-ray diffractometer with  $\text{CuK}\alpha$  radiation ( $\lambda = 1.542 \text{ \AA}$ ) with a scanning angle ( $2\theta$ ) from 0 to 50°. From the XRD data, the orientation, the lattice parameter ( $a$ ) and the grain size ( $L$ ) were determined. Applying Vegard's law, the film composition was estimated. The optical transmittance spectra were recorded at room temperature in the wavelength range 400–2000 nm using a Hitachi U3400 UV-VIS-NIR double beam spectrophotometer. The optical bandgap of the films was evaluated from the spectra. The electrical conductivity of the films was measured by the standard four-probe technique.

### 3. Results and discussion

The  $\text{Cd}_{1-x}\text{Zn}_x\text{Te}$  films prepared in the present investigation were found to be uniform and strongly adherent to the substrate surface. The thickness of the films was  $\approx 1 \text{ }\mu\text{m}$ .

The XRD spectra of the  $\text{Cd}_{1-x}\text{Zn}_x\text{Te}$  films are shown in Fig. 1. Pure CdTe films ( $x=0$ ) were found to exhibit three diffraction peaks associated with (111), (220) and (311) reflections with  $d$  values of 3.744, 2.942 and 2.295 Å respectively, of which the intensity of the (111) orientation is very predominant. The films exhibited zincblende structure with lattice parameter  $a = 6.484 \text{ \AA}$ . A shift in peak position towards higher diffraction angle ( $2\theta$ ) (from  $23.76^\circ$  to  $24.50^\circ$ ) was observed with the increase of zinc content in the films. The lattice parameter was found to decrease from  $6.484 \text{ \AA}$  ( $x=0$ ) to  $6.293 \text{ \AA}$  ( $x=0.49$ ). The absence of diffraction peaks associated with CdTe and ZnTe indicated that the  $\text{Cd}_{1-x}\text{Zn}_x\text{Te}$  films prepared in the present study were of single phase. Applying Vegard's law, the compositions of the films were estimated from the values of the lattice parameters and are given in Table 1.

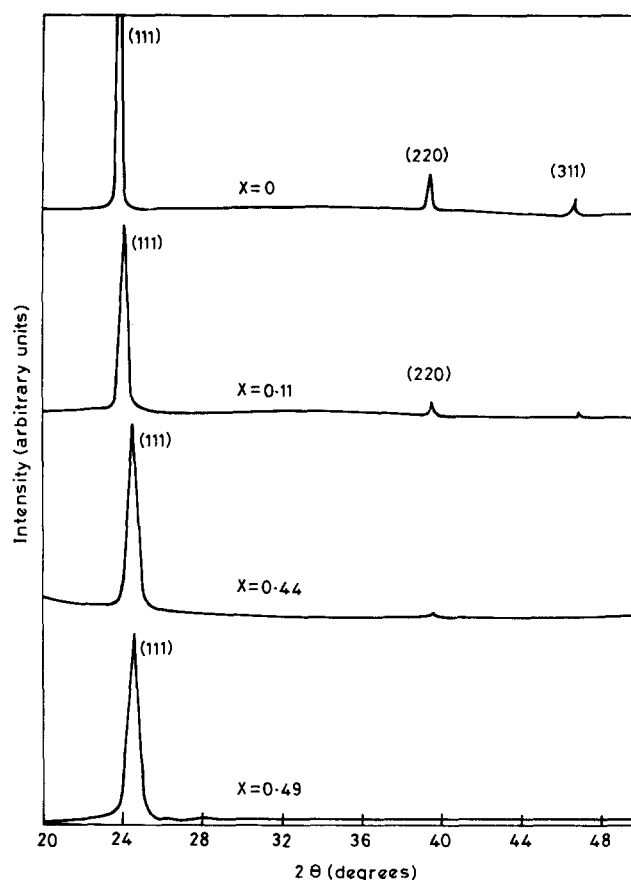


Fig. 1. X-ray diffraction spectra of  $\text{Cd}_{1-x}\text{Zn}_x\text{Te}$  films.

Table 1

Compositions, lattice parameters, grain sizes and optical bandgaps of  $\text{Cd}_{1-x}\text{Zn}_x\text{Te}$  films

Sample No.	$x$	$a$ (Å)	$L$ ( $\mu\text{m}$ )	$E_g$ (eV)
TS-02	0.0	6.484	0.174	1.48
TS-06	0.04	6.469	0.144	1.51
TS-09	0.11	6.443	0.131	1.56
TS-13	0.32	6.345	0.122	1.65
TS-17	0.44	6.317	0.110	1.72
TS-20	0.49	6.293	0.095	1.81

The grain size of the films decreased from  $0.17 \text{ }\mu\text{m}$  for pure CdTe to  $0.10 \text{ }\mu\text{m}$  for  $x=0.5$ . As the zinc content exceeds about 10%, the crystalline quality of the  $\text{Cd}_{1-x}\text{Zn}_x\text{Te}$  films decreased substantially. At higher zinc content (beyond 10%) the additional (220) and (311) phases are almost negligible, while the films showed a very strong (111) preferred orientation. Such a type of behaviour was also observed in CdZnTe films by Chu et al. [11] at higher concentrations of zinc.

The optical transmission spectra of  $\text{Cd}_{1-x}\text{Zn}_x\text{Te}$  films recorded at room temperature in the wavelength range 400 to 2000 nm are shown in Fig. 2. High transmittance in a higher wavelength region and a sharp absorption edge were observed in the films. The absorption edge

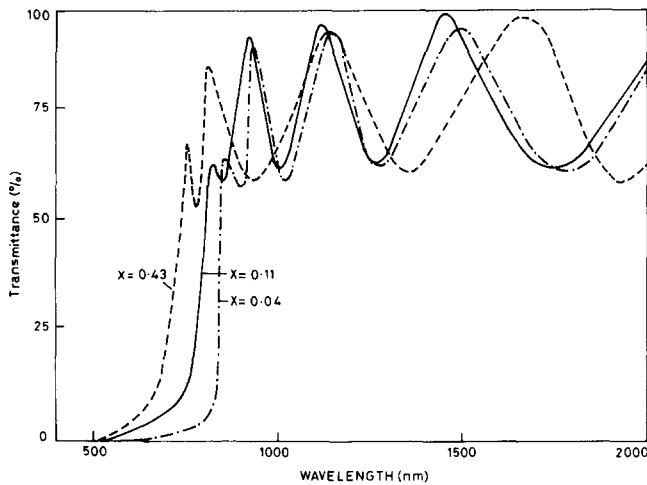


Fig. 2. Optical transmission spectra of  $\text{Cd}_{1-x}\text{Zn}_x\text{Te}$  films.

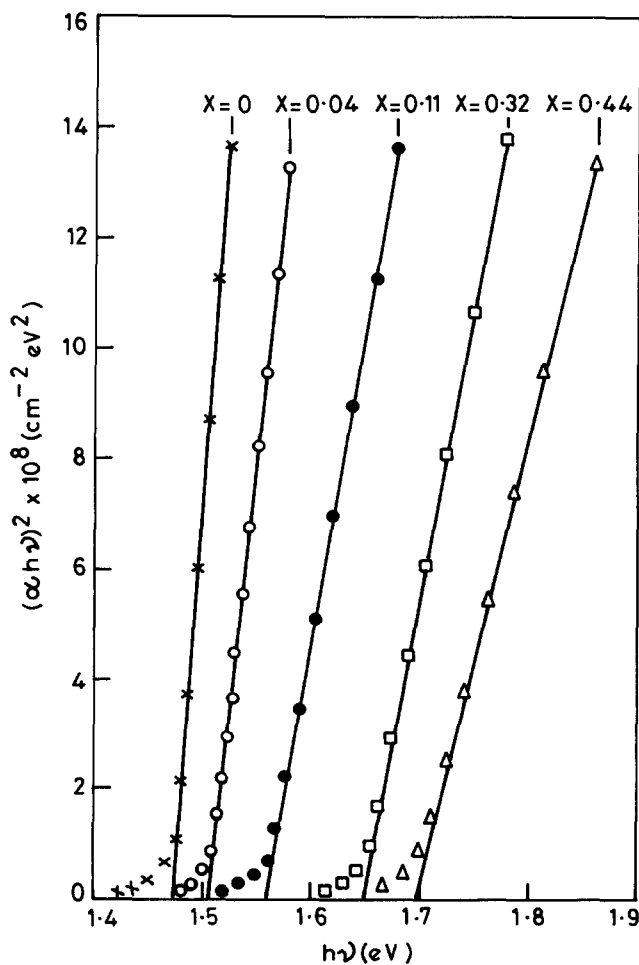


Fig. 3. Plots of  $(\alpha h\nu)^2$  vs. photon energy of  $\text{Cd}_{1-x}\text{Zn}_x\text{Te}$  films.

was found to shift towards the lower wavelength region with increasing zinc content in the films. However, the sharpness was found to decrease with increasing zinc content, which indicates the decrease of grain size with increasing  $x$ . This is also evident from the XRD data. The variation of absorption coefficient ( $\alpha$ ) with incident photon energy ( $h\nu$ ) fits the equation [14]

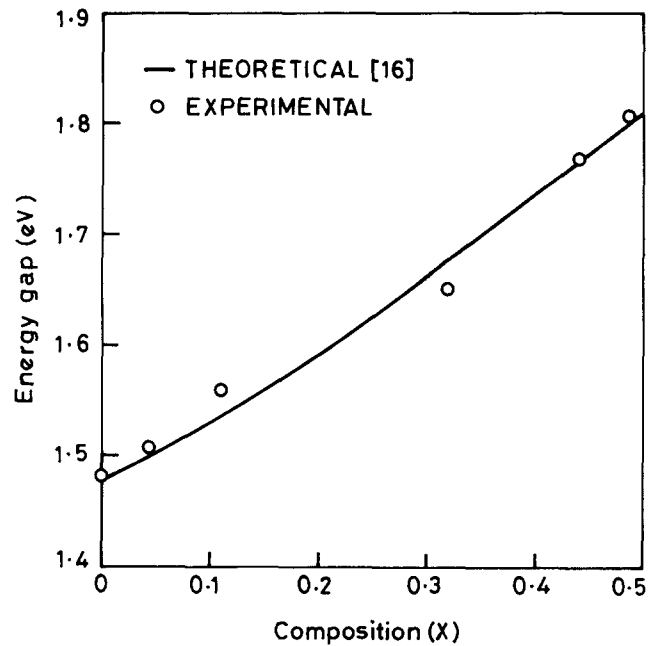


Fig. 4. Composition dependence of energy gap of  $\text{Cd}_{1-x}\text{Zn}_x\text{Te}$  films.

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

where  $E_g$  is the optical bandgap and  $C$  is a constant. The  $(\alpha h\nu)^2$  vs.  $h\nu$  plot (Fig. 3) indicates a linear dependence at the higher absorption region, suggesting a direct interband transition in the films. Extrapolation of the linear plot to  $\alpha=0$  gives the optical band gap  $E_g$ . The evaluated optical band gap of  $\text{Cd}_{1-x}\text{Zn}_x\text{Te}$  ( $x=0$ ) is 1.48 eV. With increasing  $x$  the bandgap increases to 1.81 eV for films with  $x=0.5$ . The variation of  $E_g$  with  $x$  was found to be curvilinear (Fig. 4). These results are in good agreement with the reported values [11,15].

The electrical conductivity of  $\text{Cd}_{1-x}\text{Zn}_x\text{Te}$  films was studied at room temperature. All the films exhibited p-type conductivity, which was confirmed by thermoelectric power measurements. The resistivity of pure CdTe films was about  $10^7 \Omega \text{ cm}$ . For  $\text{Cd}_{1-x}\text{Zn}_x\text{Te}$  films the resistivity decreased with increasing zinc content up to  $x=0.3$  and increased further with  $x$ . The minimum resistivity observed for  $\text{Cd}_{0.68}\text{Zn}_{0.32}\text{Te}$  films was  $10^5 \Omega \text{ cm}$ .

#### 4. Conclusions

Thin films of  $\text{Cd}_{1-x}\text{Zn}_x\text{Te}$  ( $x=0.0$  to  $0.5$ ) were prepared by co-evaporation of CdTe and ZnTe onto Corning glass substrates maintained at  $300^\circ\text{C}$ . The films were subsequently annealed in vacuum at  $400^\circ\text{C}$  for 1 h. The films exhibited (111) preferred orientation

with a variation of lattice parameter ( $a$ ) from 6.484 Å ( $x=0$ ) to 6.293 Å ( $x=0.49$ ). The optical bandgap of the films varied from 1.48 eV ( $x=0$ ) to 1.81 eV ( $x=0.49$ ). The  $\text{Cd}_{0.68}\text{Zn}_{0.32}\text{Te}$  films exhibited a direct optical bandgap of 1.65 eV and a minimum resistivity of  $\approx 10^5 \Omega \text{ cm}$ , and are quite useful as a top absorber material in the fabrication of tandem solar cells.

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