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STUDY OF THE OPTICAL PROPERTIES OF ZnTe THIN FILMS FOR USE IN PHOTOVOLTAIC CELLS

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Abstract: Zinc Telluride (ZnTe) belongs to II-VI binaries and is an important solar cell material because it has an optimum band gap ≅ 2.26eV required for the absorbance of solar cell spectrum. For the present study, ZnTe thin films were deposited onto thoroughly cleaned glass substrates kept at room temperature by vacuum evaporation. These films were annealed at temperatures of 100°C, 200°C, 300°C and 375°C for 15 minutes in air atmosphere. The optical properties of as evaporated and annealed films were then studied. A slight rise in band gap energy was observed due to annealing caused by the grain growth and improved crystallinity.

Keywords: Annealing, optical band gap, transmittance, zinc telluride.

INTRODUCTION

Zinc Telluride (ZnTe) is known as a wide band gap (2.26 eV), potentially low cost, environmentally stable, low-resistance and easily manufacturable back contact semiconducting material with low electronic affinity (3.53 eV) [Kashyout *et al*. 1997, Nishio *et al*. 2001a]. Such properties of ZnTe thin films have made them potential candidates for use in switching devices and multijunction solar cells in the recent years [Bozzini *et al*. 2000, Zenia *et al*. 2000, Ballakhadar *et al*. 2001, Nishio *et al*. 2001b, Yu *et al*. 2001, Mahalingam *et al*. 2002a,b, Klapetek *et al*. 2003, Tanaka *et al*. 2003, 2004]. Electro-optic and opto-electronic applications of ZnTe films involve resistors, transparent heating elements, electromagnetic shield coatings etc. Recent developments in solar cell technology have shown their use in CdTe, CdZnTe and HgZnTe based solar cells with a tailored band gap [Rohatgi *et al*. 1989]. ZnTe can also be used as passive layer for HgCdTe surfaces and MIS structures [Konigstein and Neumann-Spallart 1998]. All these developments caused a renewed interest in the study of ZnTe films for device applications.

ZnTe thin films have been prepared by various techniques such as closed space sublimation (CSS) [Goyal *et al*. 1997], screen-printing, thermal evaporation [Aqili *et al*. 2000], r. f. sputtering [Ballakhdar *et al*. 2001], vapour phase epitaxy [Khan 1994], molecular beam epitaxy [Tao *et al*. 1994, Camacho *et al*. 2002], hot wall epitaxy [Merchant and Cocivera 1996, Yu *et al*. 2001], metallorganic vapour phase epitaxy (MOVPE) [Nishio *et al*. 2001, Tanaka *et al*. 2003] and electrochemical deposition [Bozzini *et al*. 2000]. Each of these methods has its own limitations. Of these methods thermal evaporation is relatively a simple technique to prepare ZnTe films onto large area substrates. The present report deals with the preparation of ZnTe films with thermal evaporation on Corning glass substrates and the effects of fixed time annealing at various temperature on their optical properties such as optical transmittance, absorption, band gap energy etc.

MATERIALS AND METHODS

ZnTe thin films were prepared onto thoroughly cleaned glass (Corning 7059) substrates by thermal evaporation under a vacuum of better than 10^{-4} torr at a deposition rate of ~5.6 Ås^{-1}. The samples were then annealed in air atmosphere for 15 min. at different temperatures ranging from room temperature to 375 ºC. The optical transmittance spectra of these annealed films were recorded at room temperature (~23 ºC) by a double beam Spectrophotometer (Hitachi 2001-UV) in the wavelength range from 200 to 1100 nm.

RESULTS AND DISCUSSION

The vacuum evaporated polycrystalline ZnTe thin films were found to be smooth, uniform and had very good adhesion to the substrate surface. Fig.1 shows the optical transmittance spectrum of ZnTe thin film in the wavelength range 200nm to 1100 nm. It is obvious from Fig. 1 that the film demonstrates more than 50% transmission at wavelengths greater than 600 nm. The transmission spectrum shows interference pattern with a sharp fall of transmittance at about 560 nm at the band edge. This behaviour leads to the crystalline nature of ZnTe films. The results are comparable to those of other workers [Mahalingam *et al*. 2002b,c].

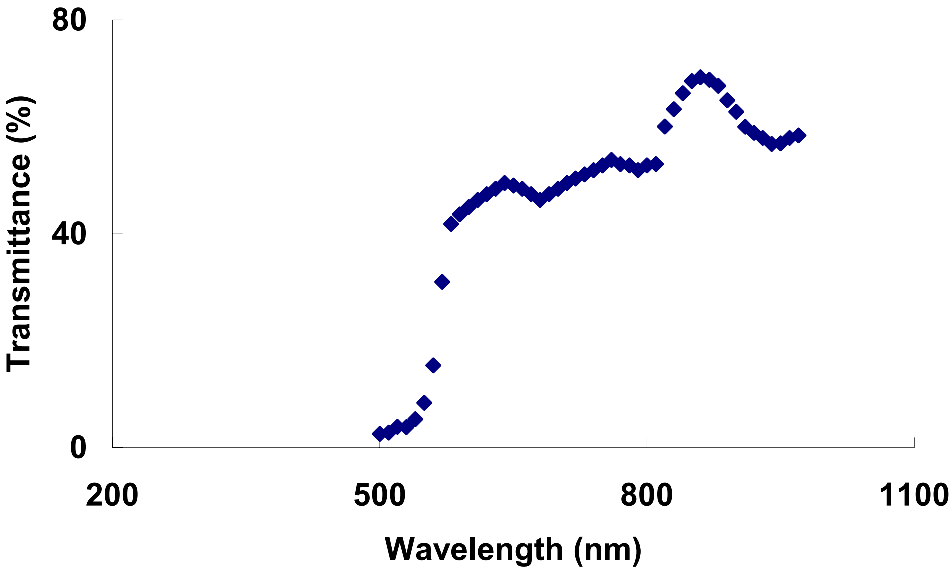

Fig.1: A graph of wavelength Vs. % transmittance for as evaporated ZnTe film.

Fig. 2 shows a plot of transmittance as a function of wavelength for a film annealed in air atmosphere at 200 °C for 15 min. The plot shows an increase in the %transmittance at higher wavelengths as compared to the un-annealed film as shown in Fig.1. The sharpness in the band edge has also improved. Such an increase in the transmittance and sharpness of band edge might be due to the grain growth and an improvement in the crystalline nature of the film [Tayan 1984, Mahalingam 2002a] caused by annealing. This result leads us to use ZnTe as a better window material.

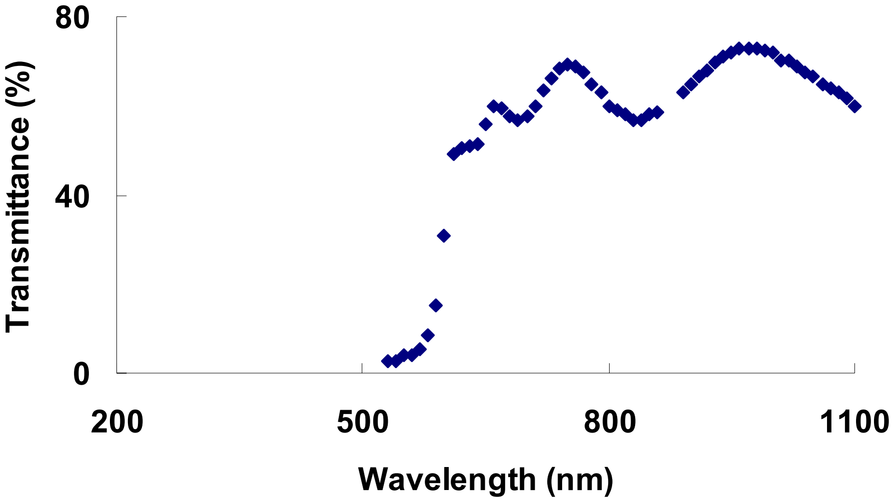

Fig. 2: A plot of wavelength Vs. % transmittance for ZnTe film annealed at 200°C for 15 minutes.

The variation of transmittance (T) with wavelength (λ) is given by the relation [Manifacier *et al*. 1976]

$$T = \frac{16 n_a n_g n^2 \exp(-\alpha t)}{R_1^2 + R_2^2 \exp(-\alpha t) + 2R_1R_2 \exp(-\alpha t)\cos(4\pi nt/\lambda)} \quad (1)$$

where n, n_a and n_g are the refractive indices of film, air and glass respectively, R_1 and R_2 are the Reflectivities or reflectances of the film and the back surface of the substrate, and α is the absorption coefficient given by

$$\alpha = \frac{1}{t}\ln\left|\frac{1}{T}\right| \quad (2)$$

The maxima and minima in the transmittance versus wavelength (T- λ) plot occur when

$$\frac{4\pi nt}{\lambda} = m\pi \quad (3)$$

where *m* represents the order number and *t* is the thickness of the film. Considering the occurance of maxima at λ_1 and λ_2 with *N* oscillations between them, the thickness *t* of the film can be evaluated by the relation [Bhattacharyya *et al*. 1992]:

$$t = \frac{N\lambda_1\lambda_2}{2\cdot[n(\lambda_1)\lambda_2 - n(\lambda_2)\lambda_1]} \tag{4}$$

Using relation (4) the thickness of the film was found to be 0.5 μm.

The optical band gap energy (E_g) of ZnTe thin films can be determined from the spectral dependence of the absorption coefficient (α), which can be written as a function of photon energy $h\nu$ by the relation [Mondal *et al*. 1987, Ringle *et al*. 1991, Bhattacharyya *et al*. 1992]:

$$\alpha = \frac{C(h\nu - E_g)^d}{h\nu} \tag{5}$$

where *C* is a constant, which is different for various transitions indicated by the values of *d*, i.e., $\frac{1}{2}, 2, \frac{3}{2}, 3$ for allowed direct, allowed indirect, forbidden direct and forbidden indirect transitions respectively. The value of *d* can be determined using Eq.(5) as follows:

$$\ln\alpha = \ln C - \ln h\nu + d.\ln(h\nu - E_g) \tag{6}$$

$$\frac{d}{d(h\nu)}(\ln\alpha) = -\frac{1}{h\nu} + \frac{C}{h\nu - E_g} \tag{7}$$

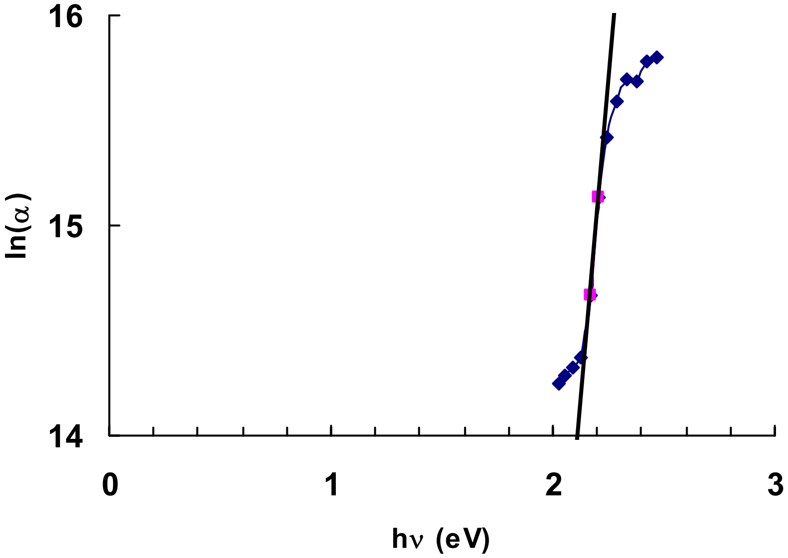

Fig. 3: A plot of ln(α) Vs. $h\nu$ for as evaporated ZnTe film.

Eq.(7) suggests that a plot of ln α versus $h\nu$ will show a divergence at $h\nu = E_g$ from which the value of E_g can be found. The value of E_g determined from the plot of ln α versus $h\nu$ comes out to be 2.11 eV (see Fig. 3). Then the slope of a plot between $\ln(\alpha h\nu)$ and $\ln(h\nu - E_g)$ yields the value of d. Such a plot is shown in Fig. 4, which depicts a value of $d \approx 0{,}57$ indicating the allowed direct transition in ZnTe thin films. Substituting $d \approx 0{,}5$ in Eq.(5) and drawing graphs between $(\alpha h\nu)^2$ and $h\nu$ for films annealed at various temperatures, the values of E_g can be obtained by extrapolating the straight line region to $(\alpha h\nu)^2=0$ (as shown in Fig. 5). The values of E_g thus obtained lie in the range 2.15 to 2.26 eV as shown in Table 1. These values of E_g are in good agreement with those of other workers [Lee 1997, Yu *et el.* 2001, Mahalingam *et al.* 2002b,c].

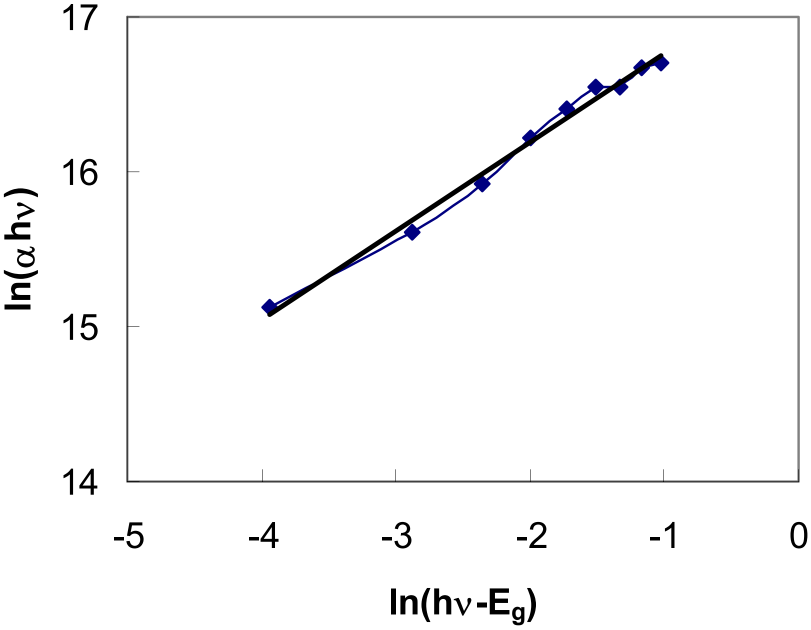

Fig. 4: Plot of ln $(\alpha h\nu)$ versus ln $(h\nu - E_g)$ for ZnTe film.

It is clear from Table 1 that E_g increases slightly with increasing annealing temperature. This increase in the band gap of ZnTe films might be attributed to the in/out diffusion of hydrogen and oxygen species into/from the film and to the formation of oxide layer on the surface of ZnTe films caused by air annealing [Jyoung 1992, Bakr 2000]. Such an increase in the band gap might also be due to grain growth and an improvement in the crystallinity. As Tayan [1984] reported that slight variation in the band gap may be due to intergrain boundary effect.

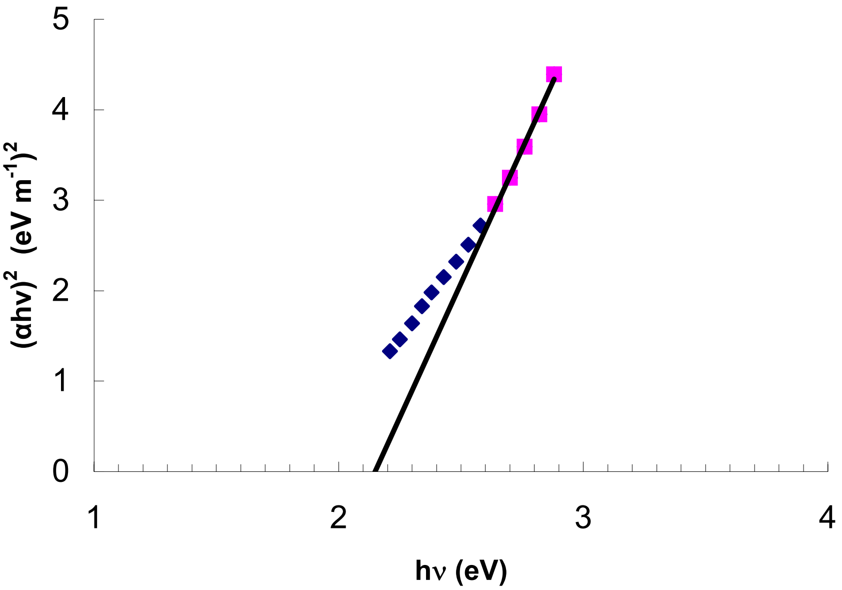

Fig. 5: A plot of $(\alpha h\,v)^2$ Vs. $h\,v$ for as evaporated ZnTe film.

Table 1: Optical band gap energy of ZnTe thin films annealed at various temperatures for 15 minutes.

Sr. No.	Annealing Temperature (°C)	Band Gap Energy (E_g) (eV)
1	Without Annealing	2.15
2	100	2.18
3	200	2.20
4	250	2.22
5	300	2.25
6	375	2.26

CONCLUSIONS

Polycrystalline ZnTe thin films were deposited onto well cleaned Corning (7059) glass substrates by vacuum evaporation at a pressure of ≈ 10^{-4} torr. The deposition rate was maintained at ≈ 5.6 $Ås^{-1}$. The films obtained were without pinholes and very well adherent with the glass substrate. Thin films of ZnTe show direct allowed transitions. Annealing of these films from 100°C to 375°C for 15 minutes in air atmosphere causes a slight rise in band gap energy. The variation of band gap (2.15-2.26 eV) has been attributed to the grain growth and improvement in the crystalline nature of the films caused by annealing.

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