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Research Article

Optical Properties of Al- and Sb-Doped CdTe Thin Films

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Nondoped and (Al, Sb)-doped CdTe thin films with 0.5, 1.5, and 2.5 wt.%, respectively, were deposited by thermal evaporation technique under vacuum onto Corning 7059 glass at substrate temperatures (T_s) of room temperature (RT) and 423 K. The optical properties of deposited CdTe films such as band gap, refractive index (n), extinction coefficient (k_e), and dielectric coefficients were investigated as function of Al and Sb wt.% doping, respectively. The results showed that films have direct optical transition. Increasing T_s and the wt.% of both types of dopant, the band gap decrease but the optical is constant as n, k_e and real and imaginary parts of the dielectric coefficient increase.

1. Introduction

Semiconductor materials like II–VI have found their way in many applications such as photovoltaic and photoconductive devices [1, 2]. Heterojunctions (HJs) have attracted intensive research interest over the last four decades [3, 4] because of their potential importance in many technological applications. Cadmium telluride (CdTe) is unique among II–VI compounds which makes it important and quite suitable for several applications as it may exhibit both n- and p-types conductivity. It is one of the few II–VI compounds that are usually used as absorbers for photovoltaic devices [5]. It is band gap of 1.5 eV, just in the middle of the solar spectrum, and processes high absorption coefficient (α) ($>10^4\,\text{cm}^{-1}$) for the visible solar spectrum [6]. One of the advantages of this material is the possibility to vary its band gap with various dopant concentrations [7].

Considerable change in optical, electrical, and mechanical properties of CdTe thin films is produced by doping. Moreover p-type and n-type doping of CdTe is easy to achieve. The elements of the first and fifth columns of the periodic table act as acceptors, and those of the third and seventh columns act as donors. Mainly Al, Ga, In, I, and Cl have been used as donors, and Li, Cu, Ag, N, P, Sb, and As as acceptors. Some of these elements show special behavior in CdTe, depending on the site they occupy in the crystalline lattice [8–15]. The maximum doping levels achievable in bulk CdTe are of around $10^{17}\,\text{cm}^{-3}$ for holes (As, P, and Li), and about $10^{18}\,\text{cm}^{-3}$ for electrons (Al, I, and In) [15].

The purpose of the present paper is to study the effect of substrate temperatures and doping percentages of Al and Sb on the optical properties of CdTe thin films. This study covered the optical energy gap, refractive index, extinction coefficient, and real and imaginary parts of dielectric constants for the prepared films.

2. Experimental Procedure

The films of CdTe are deposited by thermal evaporation technique under 10^{-6} Torr vacuum pressure using the Edward E306A coating system. Different deposition conditions were introduced to prepare the films such as substrate temperatures (T_s) at RT and 423 K and dopant weight percentage (0.5, 1.5, and 2.5) of 5 N purity of Al for n-type and Sb for p-type thin film. A high purity (99.999%) of CdTe powder from Balzer was used as a source for undoped and doped CdTe thin films deposition using molybdenum boat. The films which thickness is about 0.5 μm were grown on Corning glass substrate 7059 with a size of $1.0 \times 2.5\,\text{cm}^2$. The substrate was cleaned in a detergent, boiled in deionized water, and finally cleaned by using ultrasonic with isopropyl alcohol. After being dried, they were put at 20.0 cm distance from the evaporator source. The substrate temperature was measured and controlled using digital thermometer. The growth rate was controlled by keeping the sources temperature constant within ±5% and the deposition rate was maintained as 0.0385 μm/min. The thickness of the films was determined by optical interferometer method. The composition of the prepared films was determined using energy dispersive X-ray analysis (EDX) with the use of a Jeol JSM5600 equipment. The EDX scans results coincide with theoretical percentage values of CdTe, Al and, Sb in undoped and doped CdTe thin film [16].

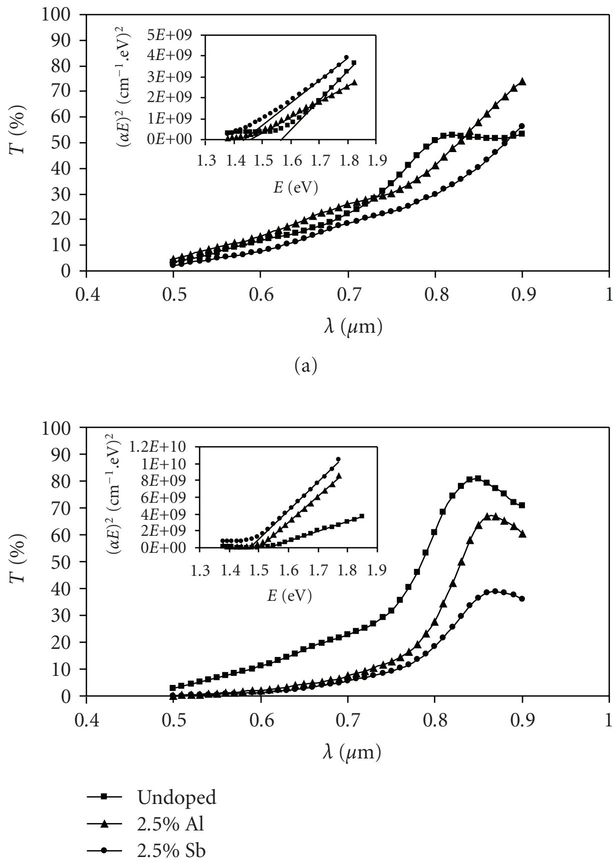
Optical transmittance spectra of undoped and doped CdTe thin films with different wt.% of Al and Sb were carried out at RT using Perkin-Elmer Lambda800-UV-VIS spectrophotometer connected with Phillips computer. The absorption coefficient (α), energy gap (E_g) and optical constants such as refractive index (n), extinction coefficient (k_e), and the real and imaginary (ε_r & ε_i) parts of dielectric constants of thin films were calculated.

3. Results and Discussion

There is a wide agreement among the researchers that the optimum approach for the determination of the optical band gap of the compound semiconductor, such as CdTe thin films, is to calculate the absorption spectra of the samples through the measurement of their transmission intensity [17].

Figures 1(a) and 1(b) show the results of such optical transmission spectrum (λ from 0.5 to 0.9 μm) for the undoped and doped CdTe films with 2.5% Al and 2.5% Sb deposited on glass substrate at substrate temperature of RT and 423 K, respectively. The spectral behavior of these films shows that the absorption edges shift to higher wavelength (lower photon energy) for films deposited at RT and 423 K after doping with Al and Sb. This indicates that the doped films have lower band gap value compared to that for undoped films. Another noticeable remark is that the transmissions for films doped with 2.5% Sb were lower than those of undoped and 2.5% Al-doped films for both deposition substrate temperatures. Also it should be noted from Figures 1(a), 1(b) that the transmission near the band edge is higher for the undoped CdTe thin film deposited at 423 K than that deposited at RT. This behavior can be attributed to the improvement in perfection of the film quality [18], and this result is in agreement with the result reported by Basol [19].

From the transmittance data and according to Tauc relation [20], $(\alpha E)^2$ versus incident photon energy (E) plots were obtained, and the graphs are presented in the inset of Figures 1(a) and 1(b). All the plots have shown straight line regions where $\alpha \geq 10^4\ \mathrm{cm}^{-1}$ indicates that CdTe has a direct allowed band gap material. This behavior is in agreement with other researchers [21–23], while Rasheed [24] had indicated that the transition in CdTe is indirect. Several



(b)

Figure 1: (a), (b) Transmission spectra of undoped and doped CdTe thin films with 2.5% Al and 2.5% Sb deposited on glass substrate at (a) RT and (b) 423 K. The inset shows $(\alpha E)^2$ versus E.

authors have observed direct and indirect optical transitions in CdTe thin films [25, 26]. This controversy in published data for E_g might be due to the variation in preparation techniques and deposition parameters.

The band gap energy (E_g) has been determined by intercepting the linear portion of the absorption curves to the photon energy axis for zero absorption coefficient ($\alpha = 0$); the values of E_g are listed in Table 1. These results showed that E_g is depending on T_s and doping concentration for both Al and Sb. Figure 2 illustrates the variation of E_g with doping percentage concentrations of Al and Sb for CdTe thin films deposited at RT and 423 K. From Figure 2 and data in Table 1 it is show that the value of E_g for undoped CdTe deposited at RT is higher than that deposited at 423 K. Similar behavior was reported by Saha et al. [25] for flash evaporated CdTe thin films. The decrease in E_g with T_s for undoped CdTe can be attributed to crystallinity improvement of films deposited at high substrate temperature. These in turn make a shift of the film band gap towards a bulk E_g value of CdTe that is, 1.51 eV. Also it can be seen that upon doping with 0.5 wt.% Al, E_g decreases from 1.57 eV to 1.54 eV at RT and from 1.54 eV to 1.52 eV at 423 K, whereas it decreases from 1.57 eV to 1.53 eV at RT and from 1.54 eV to 1.50 eV at 423 K for

Table 1: Values of E_g, k_e, n, ε_r, and ε_i for undoped and doped CdTe thin films deposited with T_s = RT and 423 K at $\lambda = 0.82\,\mu$m.

CdTe thin film	T_s	E_g	k_e	n	ε_r	ε_i
Undoped	RT	1.57	0.069	2.559	6.544	0.353
	423	1.54	0.062	2.588	6.694	0.321
Doped with						
0.5% Al	RT	1.54	0.070	2.565	6.574	0.359
	423	1.52	0.085	2.599	6.747	0.442
1.5% Al	RT	1.49	0.072	2.614	6.828	0.376
	423	1.51	0.087	2.607	6.789	0.454
2.5% Al	RT	1.46	0.096	2.699	7.275	0.518
	423	1.50	0.103	2.636	6.938	0.543
0.5% Sb	RT	1.53	0.084	2.625	6.884	0.441
	423	1.50	0.094	2.631	6.913	0.495
1.5% Sb	RT	1.48	0.107	2.642	6.969	0.565
	423	1.49	0.118	2.634	6.924	0.622
2.5% Sb	RT	1.44	0.135	2.704	7.293	0.730
	423	1.47	0.160	2.649	6.992	0.848

film doped with 0.5 wt % Sb. Upon increases the doping concentration to 2.5% Al results in a decrease in E_g to 1.46 eV and 1.50 eV for CdTe deposited at RT and 423 K, respectively. Same trend behavior is observed for increasing the doping concentration to 2.5% Sb, that is, a decrease in E_g to 1.44 eV and 1.47 eV for CdTe thin films deposited at RT and 423 K respectively. The decrease in E_g with increasing the doping concentration is due to an increase of impurity states in the gap, which causing shifting Fermi level towards valence band energy (V.B) or conduction band energy (C.B) according to dopant type, and this contributes to make the deposited film possess a narrower value of optical energy gap E_g [27]. A similar behavior has also been observed by Shehab [28] for CdTe doped with P and by Rusu [29] and Mohammed [30] for CdTe doped with Zn, while Nair et al. [31] have obtained a direct band gap of 1.42 eV for both undoped and Sb-doped electrodeposited CdTe thin films.

In general E_g value elevated with increasing T_s for films doped with percentage concentration more than 0.5% for both types as shown in Figure 2.

The extinction coefficient (k_e), refractive index (n), and the real (ε_r) and imaginary (ε_i) parts of the dielectric constant for the prepared thin films have been estimated from reflectance (R) data at λ equal to 0.82 μm using the following formula [32]:

$$n = \left[\frac{4R}{(R-1)^2} - k_e^2\right]^{1/2} - \frac{(R+1)}{(R-1)}, \tag{1}$$

where $k_e = \alpha\lambda/4\pi$.

The real and imaginary parts of the dielectric constant of the CdTe films were computed using the relation [33]

$$\varepsilon_r = n^2 - k_e^2, \ \varepsilon_i = 2nk_e. \tag{2}$$

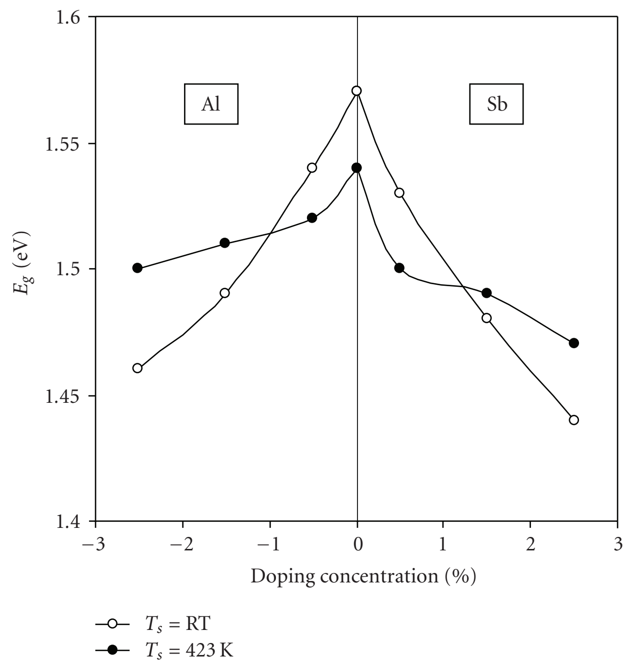


Figure 2: Variation of E_g with dopant percentage concentrations of Al and Sb.

The outcomes of these calculations are presented in Table 1. These results show that the values of k_e and ε_i are increased with increasing of T_s and doping percentage concentration of Al and Sb except that they decreased with T_s for undoped CdTe thin films. This behavior may be due to increase in absorption coefficient and it is in agreement with results shown by Saha et al. [25], while El-Shazly and El-Shair [34] showed that k_e is almost constant and independent of the substrate temperature.

The value of n for undoped CdTe film deposited at 423 K is found to be greater than that deposited at RT as shown in Table 1. The variation of n with substrate temperature may be due to the variation of the crystallographic structure of the film with the substrate temperature [30]. This behavior is in agreement with those reported by Saha et al. [25] and El-Shazly and El-Shair [34]. Also, it, can be seen from Table 1 that n for Al- and Sb-doped CdTe thin films deposited at RT and 423 K is greater than that for the corresponding undoped films which is in agreement with Saha et al. [25] for In-doped CdTe films. The data tabulated in Table 1 also shows that the value of n is increased with increasing the concentration of both type of dopant Al and Sb, but the trend of increase in n for films doped with Sb is more than those doped with Al.

The variation of ε_r with T_s and doping concentration of both types of dopant Al and Sb are the same as of n as shown in Table 1 because of the smaller value of k_e^2 compared with n^2.

4. Conclusions

Pure CdTe thin films as well as CdTe films doped with various percentages of Al and Sb were grown on the glass substrate using thermal evaporation technique. Film composition and deposition parameters were investigated for their bearing of film optical properties.

The following make the summary of the study.

(i) The films have allowed direct transition with optical energy gap lying within the range 1.44–1.57 eV.

(ii) Increasing in T_s and dopant percentage concentrations for both Al and Sb caused a decrease in the optical band gap value.

(iii) There is increase in the optical constants k_e and n with increase in substrate temperature and doped percentage concentrations except for undoped CdTe thin film, where k_e decreases with increasing T_s, and the variation of ε_r and ε_i have similar trend as for n and k_e, respectively.

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