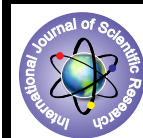


## Dispersion Parameters of Thin Cadmium Telluride Films at Different Thicknesses



### Physics

**KEYWORDS:** Thin CdTe Film, Thermal Evaporation, UV-VIS Spectra, Single Oscillator Modelw

<b>Rasha A. Abdullah</b>	University of Tikreet, College of Sciences, Department of physics, Iraq
<b>Nada M. Saeed</b>	University of Baghdad, College of Sciences, Department of physics, Iraq
<b>Hussain Kh. Al Khalid</b>	University of Tikreet, College of Sciences, Department of physics, Iraq
<b>Mohammed A. Razooqi</b>	University of Tikreet, College of Sciences, Department of physics, Iraq

### ABSTRACT

Thin CdTe films have been prepared by thermal evaporation technique on glass substrate under vacuum of about 10-5mbar. The thicknesses of the films were 2000 and 4000 ± 50Å. Absorbance spectra of the films indicate that the films have high transparency. The optical studies reveal that the transition is direct with band gap value increased from 1.51eV to 1.56eV with increasing film thicknesses. The refractive index dispersion curves obey to the single oscillator's model. The dispersion energy and single-oscillator energy varied with film thicknesses. The moments of optical spectra have studied. The infinite refractive index decreased from 2.41 to 2.05 with increasing film thicknesses.

### I. INTRODUCTION

Cadmium Telluride (CdTe) is an excellent choice for use as a semiconductor in solar panels, because it is perfectly matched to the solar spectrum [1]. Cadmium telluride provides semiconductor properties with direct band gap about 1.54 eV for hexagonal and 1.50 eV for cubic phases and its transparency allows the sunlight to pass through to the CdTe layer for wavelengths below the absorption edge. CdTe is a most promising photovoltaic material as low cost, high efficiency solar cells [1]. It is cheaper than silicon, especially in thin film solar cell technology. "When it is sandwiched with cadmium sulfide, a p-n junction photovoltaic solar cell will be formed [2, 3]. A relatively large formation enthalpy and good chemical stability of CdTe allow solar cells to be made using a wide variety of film growth methods, such as close-space sublimation, vapour transport, physical vapour deposition, sputtering, and electrodeposition. CdTe films are polycrystalline, with grain sizes ranging from 0.1 to >10 µm, depending on film thickness and deposition method and the grain boundaries tend to be benign [4]. The most efficient CdTe solar cell reported so far is a 16.5% [5]. The production of CdTe thin films has investigated for many years. The semiconductor properties of this material are suitable for application in many other optoelectronic devices, such as detectors for the infrared and x-ray [6].

### II. EXPERIMENTAL WORK

Thin CdTe films have deposited by Edward E306A vacuum system under high vacuum of about 10-5mbar on 7059 corning glass slides substrate kept at room temperature. Molybdenum boat has used as a source. Before the deposition on glass substrates, they cleaned ultrasonically with acetone, deionized water, and finally dried by air blower. The CdTe films prepared with different thicknesses 2000 and 4000 ± 50Å. The thicknesses (t) of the prepared films were measured using fizeu method. The optical properties have measured by using a double beam UV-VIS spectrophotometer type Perkin-Elmer Lambda 900. Absorbance (A) and Reflectance (R) spectra have recorded in the wavelength range 450-850 nm. The effect of film thickness on the optical properties and dispersion parameters of CdTe thin films have studied.

### III. RESULTS AND DISCUSSION

The absorbance and reflectance spectra of thin CdTe films on glass substrate measured within the wavelength range 450-850 nm at different thicknesses have illustrated in figure 1. The prepared films display high absorption at wavelength range 580-620 nm known as absorbing region. The absorption coefficient (α) of thin CdTe films determined from the following equation [7]:

$$\alpha = \frac{1}{t} \ln \left( \frac{I_0}{I} \right) \quad \text{-----(1)}$$

Where t is thickness of the film, I<sub>0</sub> and I are the intensity of incident and transmitted beam. The behavior of the absorption coefficient as a function of photon energy of thin CdTe films have illustrated in figure 2. In the shorter wavelength the absorption coefficient exhibits high values >104 cm<sup>-1</sup> which means that there is a large probability of the allowed direct transition [8]. In general, the absorption coefficient decreases with increasing the annealing temperature. The shifts of absorption coefficient spectrum to longer wavelength, red shift (smaller energies) compared to the as deposited films, similar behavior have found by Al Gahmadi et al [9]. Maximum absorption in the visible region is in the range 10-25 % for two thicknesses and this deference is due to the film thickness.

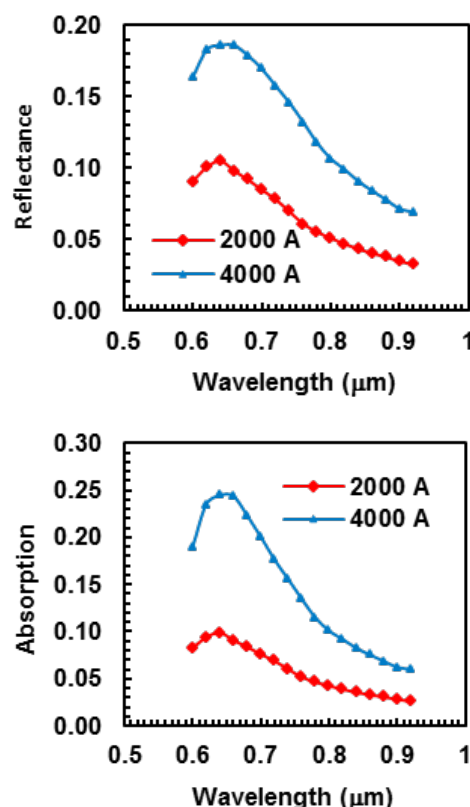


Figure 1. The absorbance and reflectance spectra as a function of wavelength of as deposited and annealed thin CdTe films at different thicknesses.

The spectral dependence of absorption coefficient in the strong absorption region is given by Tauc equation [10]:

$$\alpha h\nu = B (h\nu - E_g)^r \quad \text{-----}(2)$$

Where B is energy independent constant and r is equal to 2 or 1/2 for allowed indirect or direct transitions, respectively. A good fit between the experimental data for prepared films when  $r=1/2$ . It well known that direct transition across the band gap is feasible between the valence and the conduction band edges in k space. In this transition process, the total energy and momentum of the electron-photon system must be conserved [7]. The values of the direct optical band gap ( $E_g$ ) values of the CdTe thin films were obtained from the intercept of  $(\alpha h\nu)^2$  as function of photon energy ( $h\nu$ ) curves plotted as shown in figure 2, their values are given in Table 1. The values of the energy gap increased as thickness increased because of decreasing disorder present in the structure then redistribution of tails from band to tail, thus allows a great number of possible band to tail and from tail to tail transitions, which lead to increase optical energy gap [11]. Similar behavior has found by Al Ghamdi et al [9] and Shaaban et al [12].

The energy independent constant (B) has been obtained from the root square of the straight line in Tauc slope  $((\alpha h\nu)^{1/2}$  vs. photon energy). The B values have tabulated in Table 1. Our results show that B increased with increasing the film thickness. B is inversely proportional to non-crystallinity and width of tail states [11]. The increasing of B suggests an increase of crystallinity.

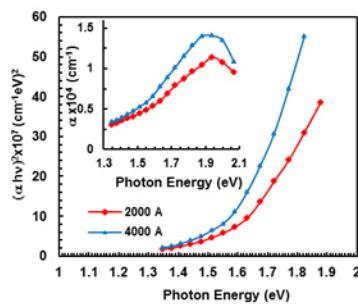


Figure 2. The variation of  $(\alpha h\nu)^{1/2}$  with photon energy and the absorption coefficient as a function of wavelength of thin CdTe films at different thicknesses.

The width of localized states inside the optical band gap of the CdTe films called Urbach tail, which related directly to a similar exponential tail for the density of states of either one of the two band edges [8]. The Urbach tail of the films has determined by the following relation [13]:

$$\alpha = \alpha_0 \exp\left(\frac{h\nu}{E_u}\right) \quad \text{-----} (3)$$

Where  $h\nu$  is the photon energy,  $\alpha_0$  is constant and  $E_u$  is Urbach energy, which refers the width of the exponential absorption edge, and it gives information about localized state in the band gap. Figure 4 shows the variation of  $\ln \alpha$  as a function of photon energy for the CdTe thin films. This behavior corresponds to optical transitions between occupied states (in the valence band tail) to unoccupied states (in the conduction band edge). Urbach energy value has calculated from the reciprocal of the slope of figure 4.

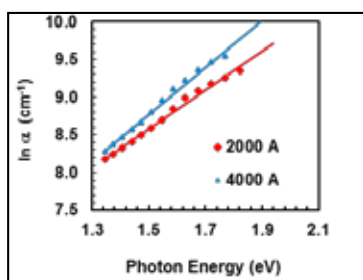


Figure 3: The variation of  $\ln \alpha$  as a function of photon energy of thin CdTe films at different thicknesses.

The  $E_u$  values change inversely with optical band gap of the films,  $E_u$  values have increased with increasing the film thickness, as shown in Table 1.

The dependence of the optical absorption coefficient with photon energy may arise from electronic transitions between localized states [10]. The density of these states falls off exponentially with energy is consistent the theory of Tauc [10], so that equation 2 can rewrite as the following:

$$\alpha = \alpha_0 \exp\left(\frac{\beta}{k_B T} h\nu\right) \quad \text{-----}(4)$$

Where  $\beta$  is called the steepness parameter, which characterizes the broadening of the absorption edge due to the electron-phonon interaction or excitation-phonon interaction,  $k_B$  is Boltzmann's constant and  $T$  is the absolute temperature. If the width of the edge related to the slope of figure 4, the  $\beta$  parameter found as  $\beta = (k_B T / E_u)$ , which is calculated by using this relationship. The absolute temperature measured at room temperature for CdTe films as shown in Table 1. The steepness parameter values suggest that the absorption edge increase as thickness increased.

Table 1: Optical parameters of as deposited and annealed thin CdTe films at different thicknesses.

t (Å)	$\alpha \times 10^4$ (cm <sup>-1</sup> )	$E_g$ (eV)	B $\times 10^7$ (cm <sup>-2</sup> /eV)	$E_u$ (meV)	B $\times 10^{-3}$
2000	0.41	1.51	110.1	383	67.5
4000	0.47	1.56	177.9	317	81.5

The theory of reflectivity of light has used to calculate the values of refractive index (n) and extinction coefficient (k). The values of n and k have calculated by using the following equations [10]:

$$k = \frac{\alpha \lambda}{4\pi} \quad \text{-----} (5)$$

$$n = \frac{\left[ \frac{((1+R) + (1+R)^2) - ((1-R)^2(1+k^2))^{\frac{1}{2}}}{(1-R)} \right]}{2} \quad \text{----}(6)$$

Where  $\lambda$  is wavelength. The values of n and k at different thickness are given in Table 2. It is clear from this table that n and k both increases with the increase in thickness similar behavior have found by Shaaban et al [12]. The physical interpretation of the variation of refractive index can be ascribed to the variation of both density and electronic structure. This indicates the dominance of density effect in the thickness dependence of refractive index. For further analysis of the optical data, a number of useful, associated relations can be derived to link the real and imaginary parts of the dielectric function and the optical constants (n, k). The following relations have used to calculate the values of the real part ( $\epsilon_r$ ) and imaginary part ( $\epsilon_i$ ) of the dielectric constant for CdTe films [10]:

$$\epsilon_r = n^2 - k^2 \quad \text{-----} (7)$$

$$\epsilon_i = 2nk \quad \text{-----} (8)$$

The values of real and imaginary parts of the dielectric constants of CdTe thin films at different thickness are given in Table 2. It can be seen that both, the real and imaginary part of dielectric constant increases with increase in photon energy at all thickness similar behavior have found by Al Ghamdi et al [9].

Table 2: optical constants of as deposited and annealed thin CdTe films at different thicknesses.

t (Å)	n	k	$\epsilon_r$	$\epsilon_i$
2000	1.52	0.027	2.32	0.08
4000	1.86	0.031	3.46	0.12

The refractive index dispersion plays an important role in optical communication and designing of the optical devices, so that

it is important to determine dispersion parameters of the films. The dispersion energy related to the optical transition strengths and optical conductivity, thus, in order to analyze the refractive index dispersion of the films, we used the single-oscillator model, developed by Didomenico and Wemple [14], which described the dielectric response for transitions below the optical gap. In terms of the dispersion energy ( $E_d$ ) and single-oscillator energy for electronic transitions ( $E_o$ ), the refractive index at a frequency can be expressed. The single-oscillator model for the refractive index dispersion expressed as follows [14]:

$$(n^2 - 1) = \frac{(E_d E_o)}{[(E_o)^2 - (\hbar\nu)^2]} \quad (9)$$

Where  $n$  is the refractive index. The dispersion energy which is a measure of the strength of inters band optical transitions. This model describes the dielectric response for transitions below the optical gap. Plotting  $(n^2-1)^{-1}$  versus  $(\hbar\nu)^2$  allows to determine the oscillator parameters. The dispersion energy and single-oscillator energy values were calculated from the slope and intercept on the vertical axis of  $(n^2-1)^{-1}$  and figure 5 illustrates  $(n^2-1)^{-1}$  as a function of the square of photon energy  $(\hbar\nu)^2$ . The dispersion energy and single-oscillator energy values are given in Table 3. The oscillator energy related with the optical band gap by an empirical formula [15]. We can see that a higher thickness means lower band gap, lower oscillator and dispersion energies. These results are very important because they are show that the optical and dispersion parameters changed with film thicknesses. The M-1 and M-3 moments of the optical spectra have obtained from the following relations [16]:

$$E_o^2 = \frac{M_{-1}}{M_{-3}} \quad (10)$$

$$E_d^2 = \frac{M_{-1}^2}{M_{-3}} \quad (11)$$

The M-1 and M-3 moments of the optical spectra values have increased as film thickness increased, as shown in Table 3.

The refractive index at infinite wavelength ( $n_\infty$ ) determined by the following relation [17]:

$$\frac{n_\infty^2 - 1}{n^2 - 1} = 1 - \left(\frac{\lambda_o}{\lambda}\right)^2 \quad (12)$$

The plot of  $(n^2-1)^{-1}$  vs.  $\lambda^{-2}$  was plotted to obtain  $n_\infty$  value of CdTe thin films. The  $n_\infty$  values have found within the range 2.42-2.05, which is decreased with increasing the film thickness, as given in Table 3.

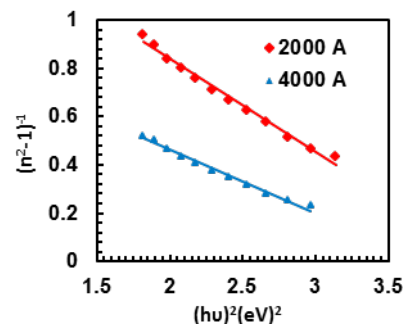


Figure 4: The variation of  $(n^2 - 1)^{-1}$  as a function of the square of photon energy for CdTe thin films.

Table 3: Dispersion parameters of as deposited and annealed thin CdTe films at different annealing temperatures.

t (Å)	E <sub>o</sub> (eV)	E <sub>d</sub> (eV)	M-1	M-3 (eV) <sup>-2</sup>	n <sub>∞</sub>
2000	1.91	1.94	0.98	0.26	2.41
4000	1.29	0.81	1.61	0.38	2.05

#### IV. CONCLUSIONS

The prepared films have direct optical band gap, which decreased as film thickness increased. Urbach energy of the films changes inversely with optical band gap. The refractive index dispersion curve of CdTe thin film obeys the single-oscillator model. The dispersion energy and single-oscillator energy for as deposited films were found to be 1.94 eV and 1.91 eV respectively changed to 0.81 eV and 1.29 eV respectively with increasing the film thickness.

#### REFERENCE

- [1] S.M. Hosseini, "Optical properties of cadmium telluride in zinc-blende and wurzite structure", *Physica B* 403 (2008) 1907–1915.
- [2] Mora-Seró, R. Tena-Zaera, J. González, V. Muñoz-Sanjós, "MOCVD growth of CdTe on glass: analysis of in situ post-growth annealing", *Journal of Crystal growth*, 262, 1-4 (2004) 19-27.
- [3] S. Deivanayagi, P. Jayamurugan, R. Mariappan, V. Ponnuswamy, "Optical and Structural Characterization of CdTe Thin Films by Chemical Bath Deposition Technique", *Chalcogenide Letters*, 7, 3, (2010) 159 – 163.
- [4] B. McCandless, J. Sites, "Handbook of PV science and technology", Wiley (2004).
- [5] Shahzad Naseem, "Preparation and Properties of Evaporation (CdTe) and all Thin Film CdTe/Cds solar cells", *Chinesse Phys. Lett.* 8, 5 (1991) 225.
- [6] A.M.D. Ede, E.J. Morton and P. DeAntonis, "Thin-film CdTe for imaging detector applications", *Nuclear Instruments & Methods in Physics Research A*, 458, 1 (2001) 7-11.
- [7] D. A. Neamen, "Semiconductor Physics and Devices Basic Principles" (Richard D. Irwin INC, 1992) p. 86, p.611.
- [8] M. H. Brodsky, "Amorphous Semiconductors" (Springer Verlag, Berlin, 1997) p.96.
- [9] A.A. Al-Ghamdi, Shamshad A. Khan, A.Nagat, M.S. Abd El-Sadek, "Synthesis and optical characterization of nanocrystalline CdTe thin films", *Optics & Laser Technology*, 42 (2010) 1181–1186.
- [10] R. E. Hummel, "Electronic properties of materials" 4th edition (Springer, New Yourk, 2011), p. 215.
- [11] N. Mott and E. Davis, "Electronic Process in Non-Crystalline Material" 2nd edition (Oxford University press, Oxford, 1979) p. 273.
- [12] E. R. Shaaban, N. Afify and A. Al-Taher, "Effect of Film Thickness on Microstructure Parameters and Optical Constants of CdTe Thin Films", *Journal of Alloy and Compounds*, 482 (2009) 400-404.
- [13] F. Urbach, "The Long-Wavelength Edge of Photographic Sensitivity and of the Electronic Absorption of Solids", *Phys. Rev.* 92, 5 (1953) 1324.
- [14] M. Didomenico and S.H. Wemple, "Oxygen-Octahedra Ferroelectrics. I. Theory of Electro-optical and Nonlinear optical Effects", *J. Appl. Phys.* 40, 2 (1969) 720-735.
- [15] G. D. Cody, "Semiconductor and Semimetals Part B; Optical Properties", Ed.: J. I. Pankove (Academic press, New York, 1984).
- [16] S.H. Wemple, M. DiDomenico, "Optical Dispersion and the Structure of Solids", *Phys. Rev. Lett.* 23, 20 (1969) 1156-1960.
- [17] F. Yakuphanoglu and C. Viswanathan, "Electrical conductivity and single oscillator model properties of amorphous CuSe semiconductor thin film", *Journal of Non-Crystalline Solids*, 353 (2007) 2934–2937.