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Analytical and Experimental Study of Structural and optical properties of thermally evaporated CdTe thin films

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ABSTRACT

CdTe Thin films were deposited on glass substrates by thermal evaporation method. The geometric thickness was calculated using interferometric method based on reflectance curve recorded with the spectrophotometer. The XRD analysis and optical characterizations of CdTe films with different optical thicknesses reveals that the structure of the films is polycrystalline with preferential orientation (111). The structure constant (a), crystallite size (D), dislocation density (δ) and strain (ε) were calculated, and it is observed that the crystallite size increases but micro-strain and dislocation density decreases with increases in thin film thickness. The overall absorbance has been increased with the film thickness and the direct band gap was obtained. It decreases with the increase in the thickness of the films.

Key word: CdTe thin film, Thermal evaporation, Absorption, Crystallite size, XRD.

دراسة تحليلية وتجريبية للخصائص الضوئية والبنيوية للأغشية الرقيقة CdTe المرسبة بالتبخير الحراري

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الملخص

رُسِّبتْ أغشية رقيقة من الكادميوم تيلورايد (CdTe) على ركازات من الزجاج بثخانات مختلفة بطريقة التبخير الفيزيائي الحراري (thermal evaporation). الثخانات الهندسية للأغشية جرى حسابها من طيف الانعكاس للأغشية، ودرست الخواص البنيوية والتوجه البلوري لهذه الأغشية بتحليل انعراج الأشعة السينية (XRD) وحُدِّدت وسطاء البنية مثل ثابت الشبيكة البلورية (a) وكثافة الانخلاعات (δ) وعامل الإجهاد (ε)، وأبعاد الحبيبات (D)، ولوحظ ازدياد الأبعاد الحبيبية ونقصان في الإجهاد المكروي وكثافة الإنخلاعات بازدياد ثخانة الغشاء المرسب. وتبيّن أن الأغشية ذات بنية مكعبة مركزية الوجوه، وحدد التوجه البلوري المفضل للغشاء والحبيبات المتشكلة عليه فكان الوجه (111) موازياً لسطح الركازة. كما استخدمنا مقياس الطيف في الدراسة الضوئية، ولاحظنا تزايداً في عامل الامتصاص بزيادة ثخانة الغشاء وتناقصاً في عرض فجوة الطاقة بازدياد الثخانة.

الكلمات المفتاحية: أغشية رقيقة CdTe، التبخير الحراري، انعراج الأشعة السينية، فجوة الطاقة، الامتصاص.

1. Introduction

Cadmium Telluride is II-V I semiconductor with a direct band gap (1.52 eV), high refractive index (2.98), and high dielectric constant [1]. Cadmium Telluride is considered at present one of the most promising materials for device applications. It has absorption coefficient in the visible range of the solar spectrum and its gap is close to the optimum value for efficient solar energy conversion [2]. CdTe is also an important semiconductor for other application such as photo-electrochemical cells, field effect transistors, detectors, photodiodes, photoconductors and photovoltaic solar cells. [3-4]. Cadmium Telluride crystals exist in two forms, cubic (zincblende) and hexagonal (wurtzite). The cubic form is stable at room temperature, while wurtzite, the less dense hexagonal form, is stable at high temperatures at atmospheric pressure [5]. Several techniques such as vacuum deposition [6], electro-deposition [7], molecular beam epitaxy [8], metal-organic chemical vapor deposition [9-10], close space sublimation [11-12] and screen-printing [13-14] have been used to produce CdTe thin film. We use thermal evaporation in this study, it is the most common method in producing thin films because its advantages are stability, reproducibility, and high-deposition rate.

2. Experimental details:

CdTe thin films were deposited on a glass substrates using thermal evaporation technique with Mo boat at temperature (150^{o}C), with different optical thicknesses of (250, 540, 744, 942) nm and we repeat the same thickness for each film and we will report some of them. The glass substrates were cleaned in ethanol before deposition.

The deposition pressure was about (7.5×10^{-6} mbar). The substrates were placed in a sample holder and kept at a distance of 18 cm from the evaporation source. The substrate holder was connected to an electric motor to rotate the substrate during the deposition to achieve uniform film. The nominal film thickness was controlled by an optical thickness monitor. In order to obtain the refractive index, extinction coefficient and their variation with different film thickness, the transmittance and absorbance measurements were taken by (Cary 5000-VARIAN) spectrophotometer, at wavelength range 175–3200 nm.

Refractive indexes and extinction coefficients of the films with different optical thicknesses were also determined from all transmittance data. The crystal structure of CdTe films was examined by X-ray diffraction (XRD). XRD study was carried out on an X-ray using (APD 2000 diffractometer) with high-intensity Cu k_α radiation with (λ = 1.5406 ˚A).

3. Results and discussion

3.1. Crystal structure

The crystallite sizes (D) were calculated using the Scherrer formula [15-16] from the Full-Width at half-maximum (FWHM) (β):

$$D = \frac{0.94\lambda}{\beta cos\theta} \quad (1)$$

Where θ is Bragg angle

The strain (ε) was calculated from formula [17]

$$\varepsilon = \frac{\beta cos\theta}{4} \quad (2)$$

The dislocation density(δ), defined as the length of dislocation lines per unit volume of the crystal, was extracted from the formula [18]

$$\delta = \frac{1}{D^2} \quad (3)$$

The lattice parameter (a) can be evaluated from the relation

$$a = d\sqrt{h^2 + k^2 + l^2} \quad (4)$$

Were h,k,l are Miller indices.

Figure.1, presents the XRD patterns of CdTe films with different optical thicknesses. By comparing the diffraction peaks position with the data base, it is found that the peak occurs at 2θ=23.7corresponding to textured (111) growth. The peak intensity increases with increasing film thickness.

Fig.2 shows the spectrum of CdTe powder exhibits sharp peaks at 2θ=23.75, 39.31, 46.43, 56.82, 62.35, 71.21, 76.30, 84.46 and 89.41 which corresponds to diffraction from (111), (220), (311), (400), (331), (422), (511), (440) and (531) planes of the cubic phase, respectively. The peak position is in a good agreement with (data file 15-0770) for cubic CdTe [19], corresponding to [25] it's found that the structure of the films which deposited on silicon substrates are more preferential and less defects than which deposited on glasses substrates.

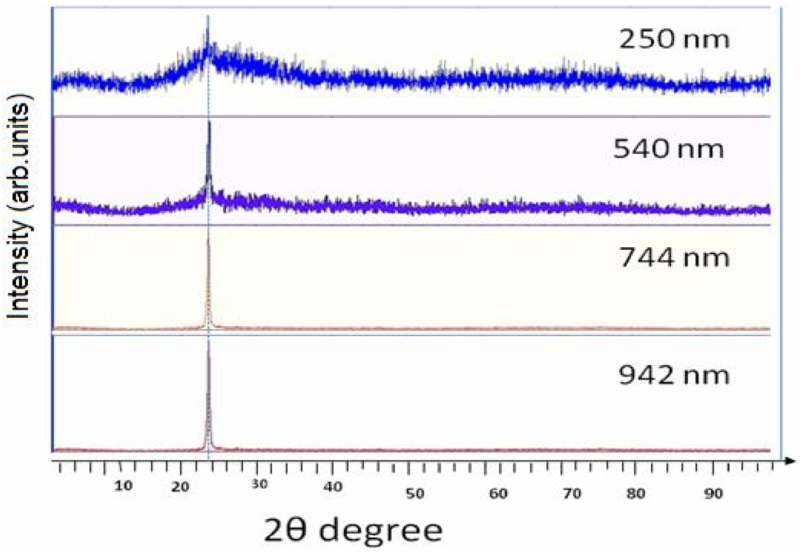

Fig.1. XRD pattern of CdTe thin films deposited at T_s=150°c with different thickness.

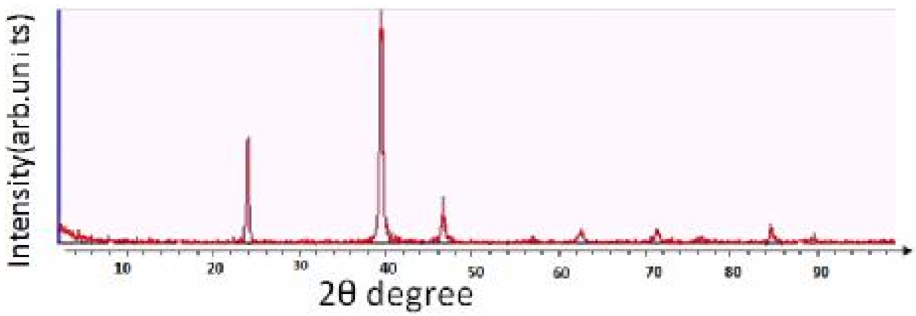

Fig.2.XRD pattern of CdTe powder

Table 1. Comparative looks of d spacing, lattice parameter, crystallite size, strain and dislocation density of the CdTe thin films of different thickness on glass substrates.

Film thickness (nm)	d spacing (nm)	Lattice parameter (a) (nm)	β (FWHM) (2θ=23.7)	Crystallite size (D) (nm)	Micro-strain(ε) $*10^{-3}$	dislocation density (δ) $*10^{-4}$ (lin/nm^2)
250 nm	0.3774	0.6536	0.71	12	3	87.7
540 nm	0.3773	0.6534	0.4	21.2	1.71	22.2
744 nm	0.3748	0.6490	0.375	22.6	1.6	19.6
942 nm	0.37511	0.6496	0.34	24.9	1.45	16.1

Table 1 shows a comparative look of the crystallite size (D), dislocation density (δ), strain (ε) of the CdTe thin films of different thicknesses on glass substrates. It is observed that the crystallite size increases but the dislocation density and micro-strain decrease with increase of film thickness on glass substrates, the decrease in micro-strain reflects the decrease in the concentration of lattice imperfections.

3.2 Optical characterizations:

3.2.1 Optical transmittance

We see at Figure 3 all the films demonstrate more than 60% transmittance at wavelengths longer than 800 nm. Below 400 nm there is a sharp fall in the %T of the films, which is due to the strong absorbance of the films in this region. It has been observed that the overall %T increases with the decrease in the film thickness. This happens due to the overall decrease in the absorbance with the decrease in film thickness. This suggests the decrease in the band-gap with the increasing thickness. For wavelength higher than 800 nm we observe thin film interference effects resulting from the over laying of light that is reflected on both sides of the thin film. This is in good agreement with the earlier investigation. [20]

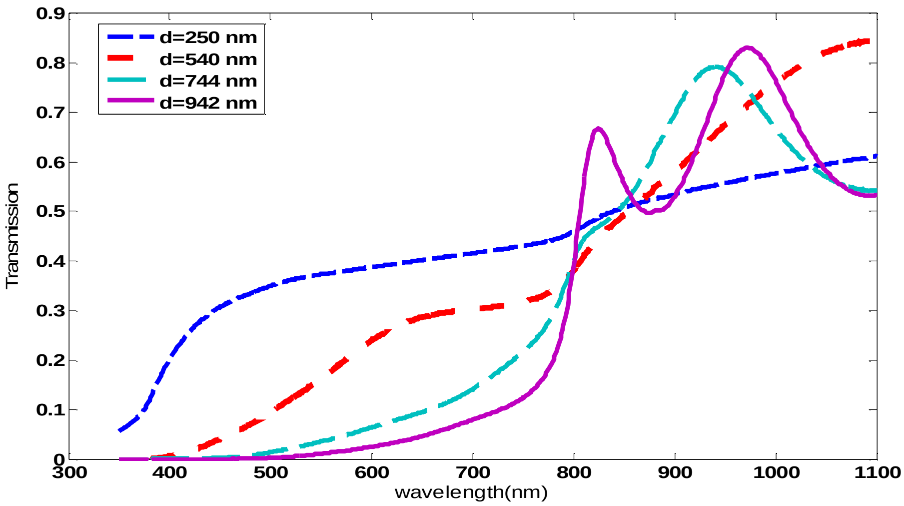

Fig.3. The optical Transmittance (T) spectra for the CdTe thin films with different thickness.

3.2.2 Bandgap

According to the theory of optical interband transitions (direct or indirect) in solids, near the absorption edge, the absorption coefficient varies with the photon energy hν according to the expression [21]

$$\alpha(h\nu)=k(h\nu-E_g^{opt})^m \qquad (5)$$

Where k is the characteristic parameter (independent of photon energy) and E_g^{opt} is the optical band gap, hν denotes photon energy and m is the number which characterizes the transition process. It is suggested that m=2 for indirect transition and m=1/2 for direct transition.

Since CdTe is a direct gap semiconductor, indirect transitions are not important. At the absorption edge, the values of absorption coefficient have been found to be in the order of $10^4 cm^{-1}$. Optical band gap of the layers maybe easily determined using equation (5) by plotting $(\alpha h\nu)^2$ versus hν in the strong absorption region (hν>1.5 ev) and extrapolating the linear portion of the plot to $(\alpha h\nu)^2=0$ fig. 4.

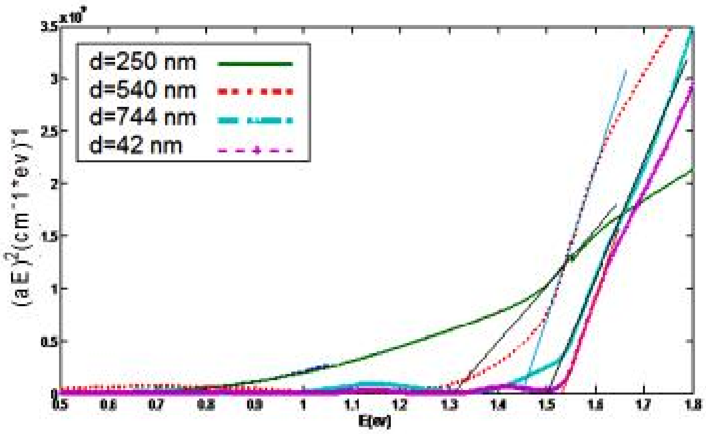

Fig. 4. Variation of $(\alpha E)^2= (\alpha hn)^2$ vs. (E)= (hn) for CdTe thin films with different thickness.

3.2.3 Bandgap versus thickness of the thin films

Figure.5 shows the bandgap versus thickness of the thin films, we can see that there is one bandgap for all thin films which is in a good agreement with [2, 16, 23, 24] and we can notice that the bandgap increases with the increases of films thickness, and that refers to the increases of crystallite size with increases of film thickness, this result is in a good agreement with XRD analysis.

Table 2. Comparative looks of Eg of the CdTe thin films of different thickness on glass substrates.

Film thickness (nm)	**Band gap E_g (eV)**
250 nm	1.31
540 nm	1.45
744 nm	1.50
942 nm	1.52

We report in Fig.5. the optical band gap of the CdTe thin films of different thickness.

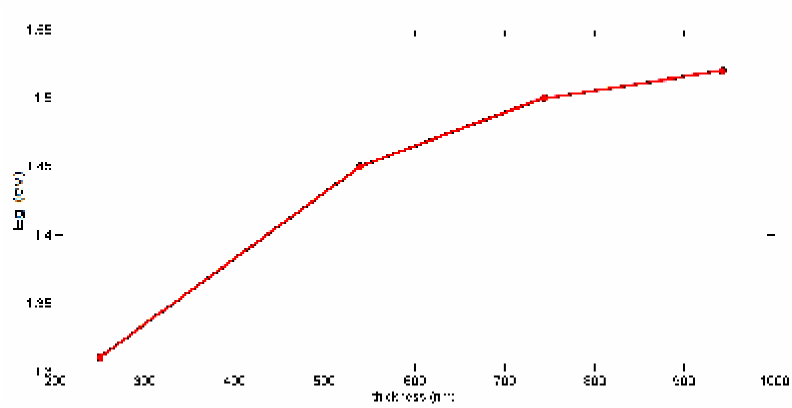

Fig. 5. Bandgap versus thickness of the thin films.

3.2.4 Extinction coefficient

The extinction coefficient can be calculated from the relation [22]:

$$K_f = \frac{\alpha\lambda}{4\pi} \qquad (6)$$

Fig.6. shows the variation of extinction coefficient with the photon energy. We see at Figure.6 a decreasing of extinction coefficient below the photon energy gap because there is no absorption in this region.

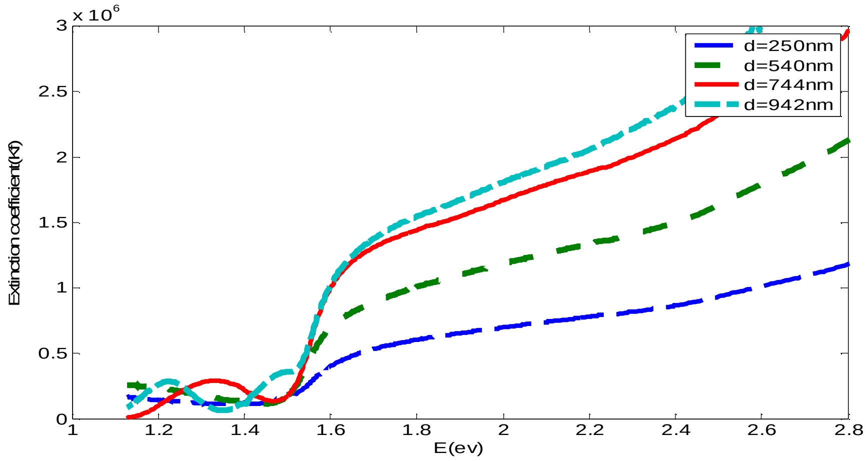

Fig. 6. Variation of extinction coefficient k_f vs. hn for CdTe thin films with different thickness.

4. Conclusions

In this work, we studied the optical and structural properties of thermal evaporated CdTe thin films on amorphous glass substrates. From XRD studies it is found that the films are polycrystalline and CdTe crystallites have zinc-blend structure.

The structure parameter of the thin films such as crystallite size (D), strain(ε), dislocation density (δ) and lattice parameter were calculated. The optical parameters such as absorption coefficient, extinction coefficient and optical band gap are calculated from transmittance and reflectance spectra. The optical transition is found to be direct and allowed with band gap energies in the range of 1.31-1.52 eV. The results are in good agreement with the earlier reported values.

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