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The Structural and Optical Properties of Zinc Telluride Thin Films by Vacuum Thermal Evaporation Technique

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Abstract

Different thicknesseses of polycrystalline ZnTe films have been deposited on to glass substrates by vacuum evaporation technique under vacuum 2.1×10^{-5} mbar. The structural characteristics studied by X-ray diffraction (XRD) showed that the films are polycrystalline and have a cubic (zinc blende) structure. The calculated microstructure parameters revealed that the crystallite size increases with increasing film thicknesses. The optical measurements on the deposited films were performed in different thicknesseses [400 , 450 and 500]nm, to determine the transmission spectrum and the absorption spectra as a function of incident wavelength. The optical absorption coefficient (α) of the films was determined from transmittance spectra in the range of wavelength (400-1100) nm. The dependence of absorption coefficient, on the photon energy showed the occurrence of a direct transition with band gap energy from 2.24eV to 1.92eV (for ZnTe films of different thicknesseses), where with high film thicknesses there are several energy levels resulting in several overlapping energy bands in the band gap of these films. The overlapping energy bands therefore tend to reduce the energy band gap, resulting in lower band gaps for thicker films.

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Introduction

Polycrystalline thin films of II-VI compound semiconductors have reasonable importance in electronic and optoelectronic devices fabrication due to their high absorption coefficients and low fabrication costs [1]. Amongst the wide band gap II-VI semiconductor materials, Zinc Telluride (ZnTe) is the most attractive material and finds several applications in the field of device electronics [2]. In addition, it possesses many interesting properties, such as a wide energy band-gap, large photoconductivity, and high excitonic binding energy high-quality, nanostructured ZnTe films are widely used in various fields such as light emitting diodes, photodetectors, laser diodes , gas sensors, field emission and solar cells[3]. There are several reports on deposition of polycrystalline ZnTe thin films by various techniques ,most of the previous research has focused primarily on the structural, electrical and optical properties of ZnTe both in the form of bulk crystals and sub-micron thin films [4]. In the present work, we focus on the study of the influence of the thicknesses on optical properties of ZnTe.

Experimental part

Thin films of high purity (99.999) ZnTe was used as a source material for the evaporation. With [400,450 and 500] nm thicknesses were deposited on glass substrate by thermal vacuum evaporation using (Edwards – Unit 306) system with 2.1×10^{-5} mbar. The thicknesses of films were determined with (Precisa -Swiss) microbalance by using weighing method and with deposition rate about (1.2 ∓ 0.1) nm/sec. The material was placed into molybdenum boat with a small dimple at the center to act as a point source. The boat was heated indirectly by passing current through the electrodes. Cleaned glass slides were used as a substrate. These glass slides were cleaned with chromic acid, ultrasonic cleaner, soap water, distilled water and then with acetone. The material evaporated in vacuum at room temperature onto cleaned glass substrates with $(2.5 \times 2 \times 1)$ cm^{3}size. The distance between the substrate and the boat is (18) cm. After reaching high vacuum in the vacuum chamber, slowly current was applied to the electrodes to heat the substance. Optical transmission measurements were performed with (UV/Visible 1800 spectrophotometer). The band gap (Eg) and optical constants of the transparent films were determined from the optical transmission spectra.

Results and Discussion
Structural properties

The structure of ZnTe thin films of different thicknesses were analysed by X-ray diffraction system uses CuKα radiation source, which has wavelength 1.5418 Å. as shown in Fig. (1). In ZnTe films only one prominent peak was observed along (111) plane .The films are crystalline in nature and have cubic structure and the corresponding values of inter planar spacing, d_{hkl} ((hkl) are Milles indices), were calculated from the Bragg equation [5]

$$2d \sin \theta = n\lambda \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (1)$$

Where θ is the angle of incidence and λ is the wavelength of the X-rays, n is an integer and it is the order of reflection, and d_{hkl} is the distance between the lattice planes . And we determined lattice parameter, *a*, from relationship

$$\frac{1}{d^2} = \frac{(h^2+k^2+l^2)}{a^2} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots (2)$$

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compared with the standard values (American Standard Testing Materia)(ASTM) [6]. The sizes of the crystallites were also determined from X-ray diffraction data using the Scherer's relation

$$(C.S) = \frac{0.94\,\lambda}{\text{ß}\cos\theta} \dots\dots\dots\dots(3)$$

Where λ is wavelength of radiation, β is full width half maxima and θ the diffraction angle. And the dislocation density (δ) of films was estimated using the equations

$$\delta = \frac{1}{(C.S)^2}\dots\dots\dots\dots\dots\dots(4)$$

The crystallite size (**G.S**), dislocation density (δ) and lattice spacing are calculated and presented in Table (1).

It is observed from XRD pattern of films that intensity of (111) peak and its grain size have increased with the increase of film thicknesses from 400 to 500nm, the improvement in crystallinity is due to fast growth of crystallite , increased ability of atoms to move towards stable sites in the lattice [7and 9] and due to the decrease in lattice defects among the grain boundaries with the grain size increase [10]. The dislocation is imperfection in the crystal which is created during growth of thin film. The dislocation density decreases with increase of film thicknesses due to fast growth of crystallite [11].

Optical properties

Fig.(2) shows the optical transmittance spectra with wavelength from 300nm to 1100 nm of the ZnTe thin films with different thicknesses, It is shown that the transmission of these films increases rapidly within the range 500-900nm reaching the maximum value. After this maximum, the transmission approximately remains constant at near-infrared wavelengths. Also from these curves one can see the transmittance of the thin films varies between 56% - 73% , maximum of 73% being reached for ZnTe thin films with lower thicknesses (400nm). With increasing the thicknesses (from 400nm to 500nm) the spectra show decrease in the transmission. There is a sharp fall from 73% to 56% in the transmittance as the thicknesses rises from 400 to 500 nm; due to increase in the density of the film. Due to highly transparent in visible and IR region [12,13]. The transmittance spectra of the films decrease as film thicknesses increases, which is identifyies a good crystallinity of obtained thicknesses [14, 15].

From figs.(3) and (4) can see vice versa in the absorption spectra and reflectance spectra of ZnTe films deposited onto a glass substrate, the absorption edge shifts to higher wavelength for higher thicknesses and it changes with film thicknesses .The reflectance spectra of films are shown in Fig.(4). It is observed that the average reflectance film increased rapidly in visible region and then decreases with the increase of wave length from the range of (800 to 1100) nm with the increase in thicknesses. The change in the reflectance of the films suggests that the refractive index films is changed where the shift of transmittance and reflectance indicates changes in the film thicknesses.

The ability of a material to absorb light is measured by its absorption coefficient and it is a very strong function of the photon energy and band gap energy [16]. The variation of the optical absorption coefficient with photon energy for various thicknesses is shown in Fig.5. The absorption coefficient (α) of a film of thicknesses (t) can be calculated from the transmittance spectrum using the relation [16]:

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$$\alpha = (2.303)\,\frac{A}{t} \quad\text{.................................. (5)}$$

Where, A: is the absorbance, which is calculated from the relation {A=log (1/T)}, (T) is the transparence. The calculated values of absorption coefficient are in the order of 10^4 cm^{-1}. The variation of optical absorbance with wavelength reveals a high absorption of energy at shorter wavelength and vice versa. The spectra also confirms that with increasing film thicknesses the absorption effect decreases exponentially due to the effect of index of refraction of films [17].

The fundamental absorption, which corresponds to electron excitation from valance to conduction band, can be used to determine the nature and value of the optical band gap. The optical band gap of the ZnTe thin films is calculated using the expression [18]:

$$(\alpha\, h \vee) = B(h \vee - Eg)^r \quad\text{··················(6)}$$

Where, B is constant, α [cm^{-1}] is the absorption coefficient, h$\vee$ is the photon energy and Eg [eV] is the optical band gap. The parameter (r) is an index related to the nature of the material which is determined by the optical transition involved in the absorption process, it specifies the allowed direct (r = 1/2) and indirect transition (r = 2) in the electronic band structure. The optical band gap energy Eg was obtained from the intercept on the photon energy axis after extrapolating of the straight line section of the curve of (α h $\vee$)^2 versus (h $\vee$) plot as shown in Fig.(6) .

Due to increase in film thicknesses the results are decrease of energy band gap from 2.24eV to 1.92eV, the individual levels of free atoms will broaden the energy bands and create overlapping levels. This occurs when atoms become closer to each other. Hence, with high film thicknesses there are several energy levels resulting in several overlapping energy bands in the band gap of these films. The overlapping energy bands therefore tend to reduce the energy band gap, resulting in lower band gaps for increment on films thicknesses [19].

Conclusions

Different thicknesses of polycrystalline ZnTe films have been deposited onto glass substrates at room temperature by vacuum evaporation technique. From XRD studies it was found that the film is polycrystalline with only one prominent peak was observed along (111) plane, having the zinc blende structure .The calculated microstructure parameters of the ZnTe thin films such as crystallite size (***G.S***) showed that the size of crystallites increases with the increase of the film thicknesses, The optical band gap decreases with the increase of the film thicknesses. The increase of ($E_g{}^{opt}$) for direct transition may be attributed to the increase in crystallites size. The increase of grain size with thicknesses can be attributed to the improved crystallinity. The improvement in crystallinity is due to increase ability of adding atoms to move towards stable sites in the lattice.

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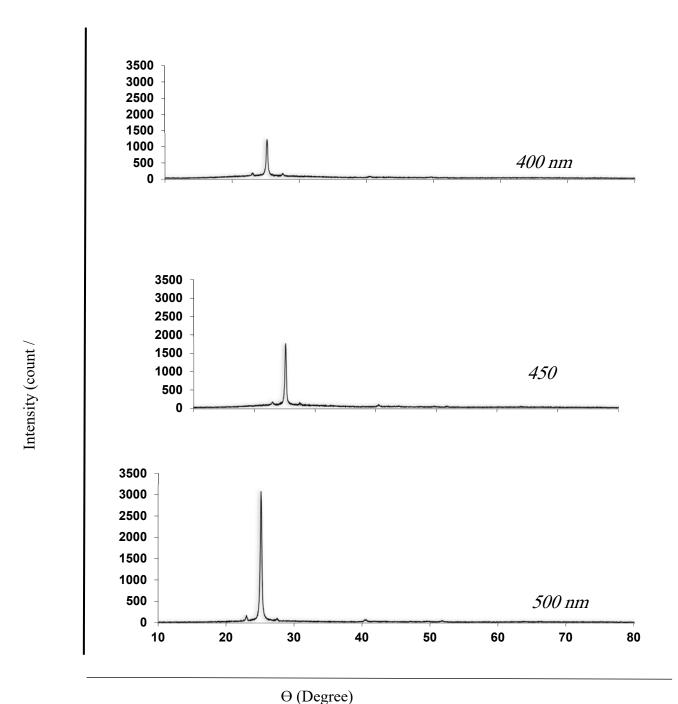
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Table 1. XRD analysis of ZnTe thin films

Films thicknesses ZnTe (nm)	2 θ	d (Å)	a(Å)	G.S nm	δ x 10^{15} (m^{-2})
400	25.2530	3.53386	6.10313	26.4103	1.4337
450	25.2068	3.53023	6.11414	31.411	1.0135
500	25.1788	3.53386	6.12082	31.939	0.9802

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Figure(1).   XRD of ZnTe thin films

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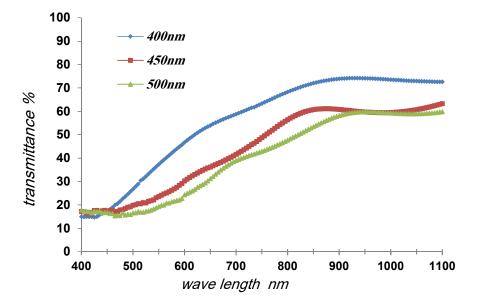مجلة إبن الهيثم للعلوم الصرفة و التطبيقية

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Figure. (2): Transmittance spectra of ZnTe thin films with different thicknesses

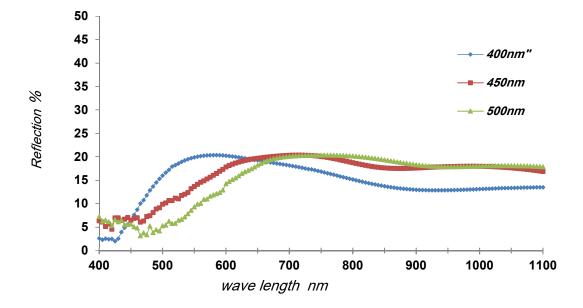**Figure. (3): Absorption spectra of ZnTe thin films with different thicknesses**

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Figure. (4): Reflectance spectra of ZnTe thin films with different thicknesses

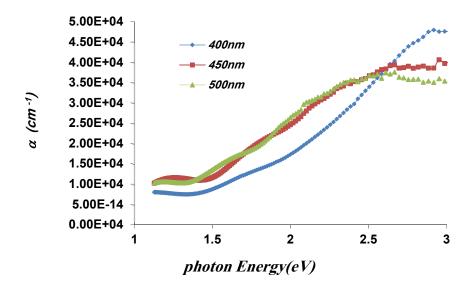**Figure.(5): Variation of absorption coefficient as a function of photon energy of ZnTe thin films with different thicknesses**
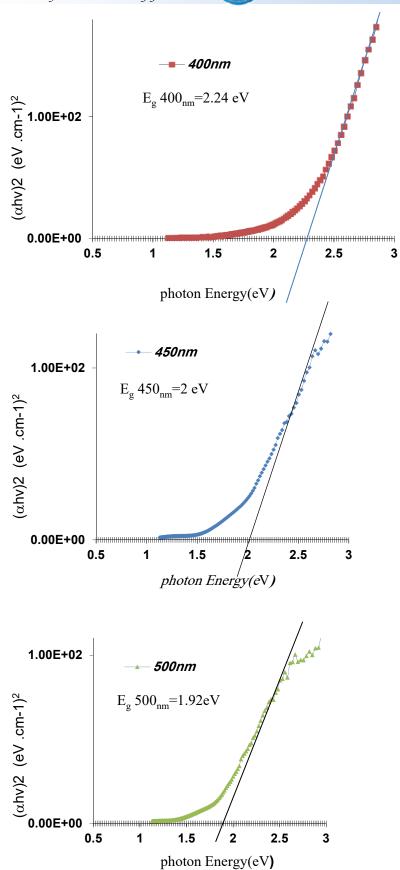
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Figure (6): Variation of (αhv)² with photon energy of ZnTe thin films with different thicknesses

الخواص التركيبية والبصرية لاغشية ZnTe والمحضرة في الفراغ بتقنية التبخير الحراري

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الخلاصة

رسبت اغشية ZnTe المتعددة التبلور على ارضية من الزجاج وباسماك مختلفة باستعمال تقنية التبخير الحراري بالفراغ تحت ضغط mbar $2.1x10^{-5}$ وبدرجة حرارة الغرفة . تم دراسة الخواص التركيبية من خلال حيود الاشعة السينية قد اظهرت النتائج بأن الاغشية متعددة التبلور وهي من نوع ركاز الزنك (Zinc-blende structure) وهوالتركيب المكعبي. وكشفت الحسابات التركيبية للحجم الحبيبي بأنه يزداد مع زيادة سمك الاغشية .وحددت القياسات البصرية للاغشية المرسبة باسماك مختلفة [nm 500 and 400, 450] طيف النفاذية والامتصاصية كدالة للطول الموجي ,ومن طيف النفاذية لمدى الاطوال الموجية nm (400-1100) تم تحديد معامل الامتصاص البصري . وكان الانتقال المباشر لفجوة الطاقة من 2.24eVالى 1.92eV (لاغشية ZnTe وللاسماك المختلفة) التأثير في اعتماد معامل الامتصاص في فجوة الطاقة والاستدلال على فجوة الطاقة من سمك الغشاء .

الكلمات المفتاحية : الاغشية الرقيقة ZnTe , القياسات البصرية , التبخير الحراري , الخواص التركيبية