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Some Optical Properties of (ZnTe) Thin Films Prepared by Thermal Evaporation Technique on a Glass Substrate

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Abstract

Thin films of Zinc telluride (ZnTe)were deposited by thermal evaporation technique on a glass substrate. The optical obtained data were analyzed using numerical analysis program which showed that the transition mechanism involved indirectly allows transition, since the best line dependence is obtained from a plot of $(\alpha h\nu)^{0.5}$ versus photon energy $(h\nu)$ .The band gap decreased from 1.15 to 0.96 eV as the substrate temperature varied from 410 to 510 K. Such behavior is attributed to unsaturated defects, which are confirmed by XRD examinations.

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Keywords: Thin films, transition mechanism, Zinc telluride.

Introduction:

Zinc telluride (ZnTe) is one of the important semiconductor materials of II–VI group because of their extensive potential applications in different opto-electronic devices [1,11,12,14,16,21,28,30]. ZnTe thin films are widely used in modern technologies of solid-state devices(light-emitting diodes, solar cells, photo detectors, etc.) because of its characteristics, namely large energy band gap, low resistivity, high transparency in visible spectral domain, etc. [3,9]. In series of previous papers [2,11,19], some electronic transport and optical properties of vacuum evaporated ZnTe thin films were studied.

Zinc telluride thin films grown at room temperature and higher substrate temperatures were found to be polycrystalline and have large number of grain boundary potentials as well as other native defects [7,10,13,20,22]. The potential barrier is localized in the grain boundaries and the conductivity is modified by externally applied fields, this is called the Poole–Frenkel conductivity. The electrical transport mechanisms in ZnTe thin films have been investigated in [5].

Some studies on Frenkel pairs of two sub-lattices ZnTe and on the predominance of Poole–Frenkel mechanism in the photo conductivity of ZnTe thin films at room temperature were reported in[29]. ZnTe has direct large band gap, it is used as a window material in hetero junction cells [23,25]. The dielectric constant and the energy gap were found to be 8.5 and 2.3 eV respectively in [4].

In this paper, the attempts have been made to determine the optical transitions types and study the substrate temperature on the optical energy gap of ZnTe thin films.

Experimental details

ZnTe thin films were prepared by thermal evaporation under vacuum (10^{-4} Pascal) of ZnTe polycrystalline powder (99.999% purity). Thin films of 500 nm thickens deposited onto optically flat quartz and glass substrates. The deposition rate was kept constant at 6 nanometer per second. The film thickness was measured after preparation by multiple beam Fizeau fringes [26]. Tantalum boats were used as source heater. The substrate temperature was measured using Achromel-alumel thermocouple. The substrate temperature varied from 298 to 510 K.

Transmittance, T and reflectance, R of films were determined at normal incidence in the spectral range 300–2500 nm by means of a double beam spectrophotometer(JASCO.V-570, UV–VIS–NIR).

Results and discussion

Five samples of ZnTe thin films in the thickness range 500–520 nm were selected to study the effect of the substrate temperature on the energy gap E_g , and the type of the optical transitions.

For this purpose both the transmittance, and the reflectance, were measured for each sample in the spectral range 300–2500 nm, at substrate temperatures 410, and 510 K.

Fig. 1 shows the spectral distribution of transmittance and reflectance for ZnTe thin film of thickness 500 nm deposited at substrate temperature of 510 K as a representative example. It is clear from Fig. 1 that the values of (R+T) < 1 in the range of spectrum is (300 – 700 nm), this behavior indicates that, the absorption exists in this range.

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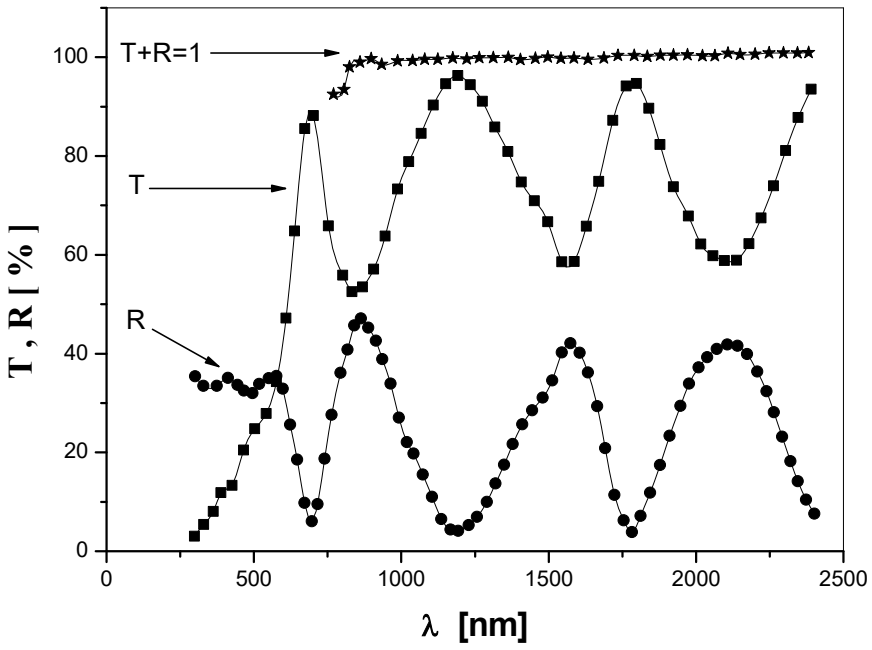


Fig. 1. Shows the spectral distribution of transmittance, T, reflectance, R and T + R for ZnTe thin film of thickness 500 nm deposited at substrate temperature of 510 K as a representative example.

Fig. 2 shows that the effect of substrate temperature on the transmittance in the visible region was also investigated. The transmittance spectra of the films were deposited at substrate different temperatures. The absorption edge move towards the ultraviolet region as the substrate temperature increases. The shift of the absorption edge to the longer wavelength region is caused by decreased Burstein–Moss shift [15,31] caused by the increase in charge carrier concentration and the occupation of electrons to low energy levels.

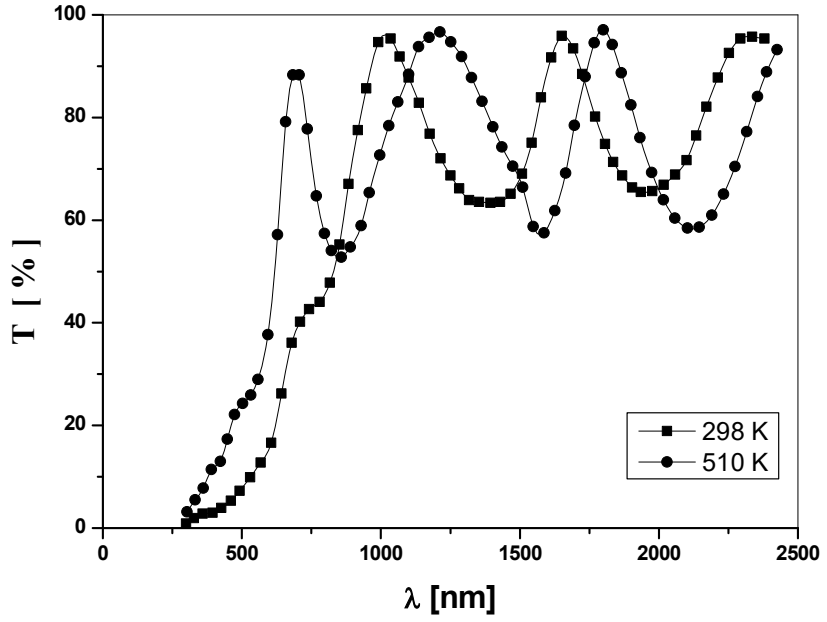


Fig. 2. Shows the effect of substrate temperature on the spectral distribution of transmittance for ZnTe film of thickness 500 nm as a representative example.

the optical absorption coefficient α was calculated using the relation[17]

$$\alpha = \frac{(2.303)}{d}\log\left(\frac{1}{T}\right) \quad (1)$$

where d is the thickness of the film and T is the transmittance. The various types of transitions give rise to different frequency dependencies of the absorption coefficient near the fundamental absorption edge. The absorption coefficient is given by [17, 24]**:**

$$Y = (\alpha h\nu) = A(h\nu - E_g)^r \quad (2)$$

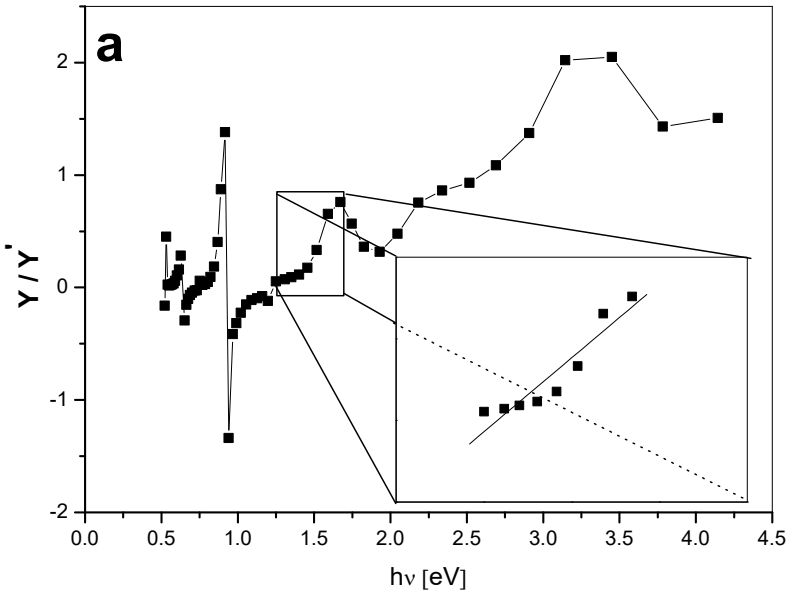
where A is a constant, E_g the semiconductor band gap and **r** depends on the kind of optical transition that prevails. Specifically, **r** is 1/2; 3/2; 2 and 3 when the transition is directly allowed, directly forbidden, indirectly allowed and indirectly forbidden, respectively. In order to determine the type of transition we have to test the above equation to find the relation which gives a straight line at higher energy range above the absorption edge. Instead of presuming the value of **r** we can determine it as follows **[**18**]** from equation (2).

$$Y' = \frac{d(\alpha h\nu)}{d(h\nu)} = Yr(h\nu - E_g)^{-1} \quad (3)$$

And we have,

$$\frac{Y}{Y'} = \frac{(h\nu - E_g)}{r} \quad (4)$$

To deduce the type of transition, Y' will be achieved utilizing numerical analysis program and then we plotted (Y/Y') versus $h\nu$ for the studied films as shown in Fig. 3. The slope of the straight line indicates that $r = 1.96$. This means that the films obey Tauc's [27] relation for the directly allowed transition. Plots of $(\alpha h\nu)^{0.5}$ vs. photon energy $h\nu$ are represented in Fig. 4. Values of E_g were obtained from the extrapolations of the linear portions of the plots. The optical energy gaps are determined to be about 1.15 and 0.96 eV for deposited and heating substrate films respectively. Here we can say that, the optical gap is expected to decrease due to the diminution of disorder and defects in the structural bonding. On the other hand, several possible reasons that contribute to a decrease in optical energy gaps have been postulated in reference [6]. In the present study, the decrease of optical band gap ,description in Fig. 4, could be attributed to the presence of unsaturated defects, which decrease the density of localized states in the band gap and consequently decrease the optical energy gap.



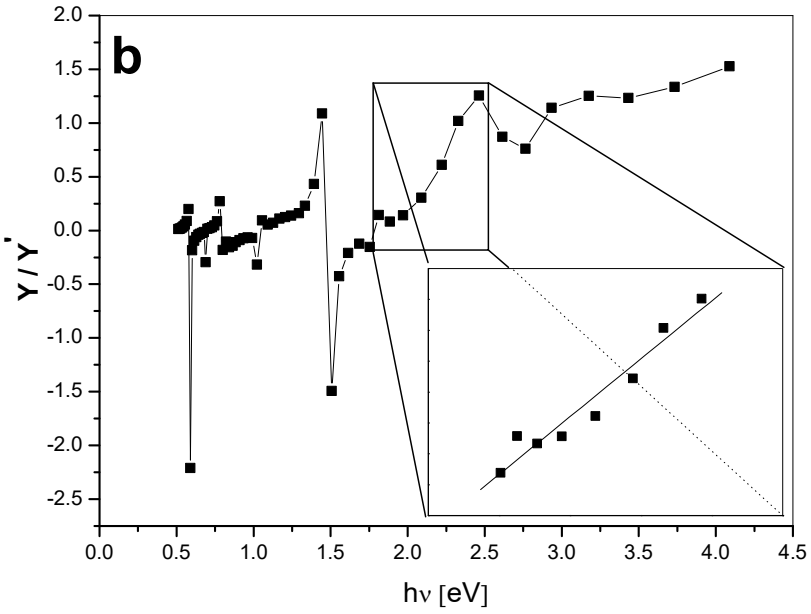


Fig. 3: (Y / Y') **as a function of photon energy for ZnTe thin films (a) before heating substrate (b) after heating substrate**.

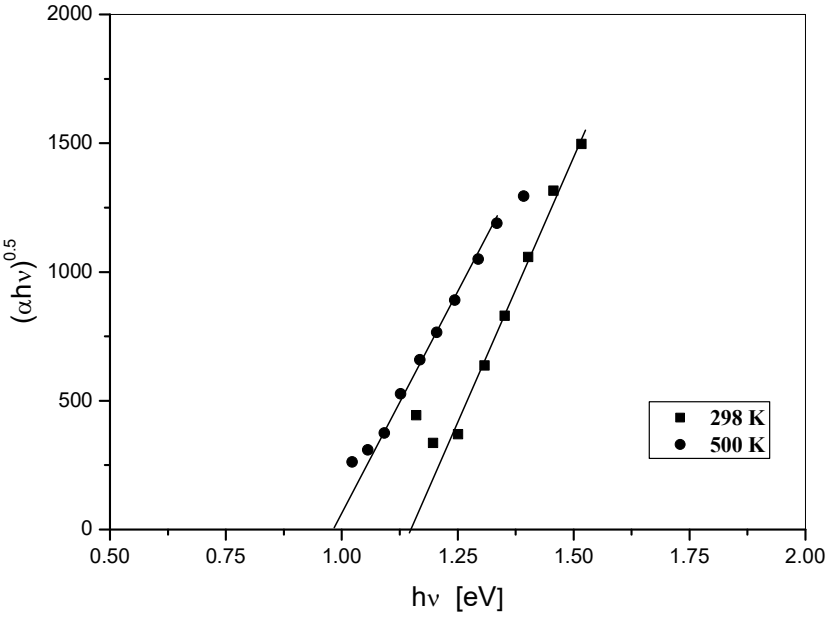


Fig. 4: $(\alpha h\nu)^{0.5}$ **as a function of photon energy for ZnTe thin films (■) before heating substrate (●) after heating substrate**

These results are confirmed by XRD examination. In a representative example, **Fig. 5.** the XRD patterns of ZnTe thin films indicate that the studied samples are polycrystalline and have a cubic structure.

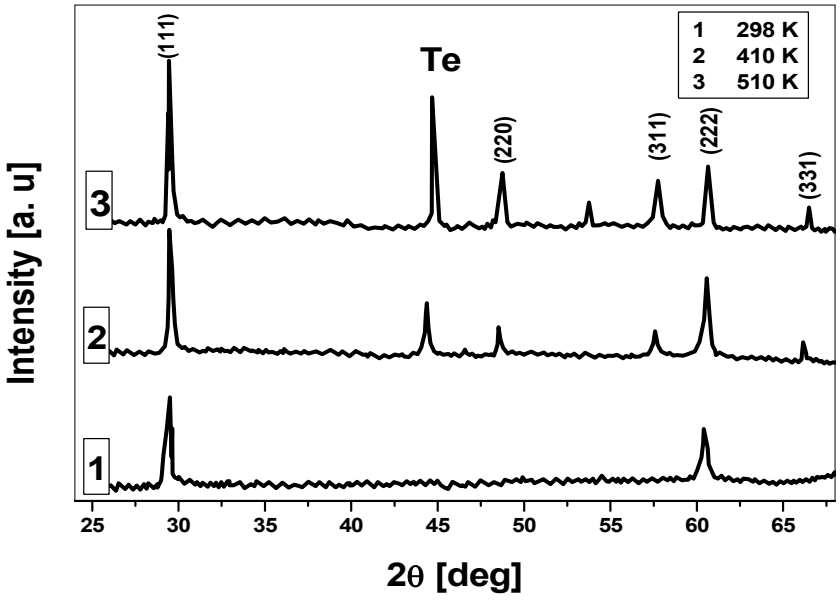


Fig. 5: XRD patterns for ZnTe thin film prepared at different substrate temperature

Different diffraction peaks were identified and the corresponding values of inter planar spacing, d_{hkl} (h, k, l are Miller indices), were calculated from the Bragg's equation [32]:

$$2d_{hkl}\sin\theta = n\lambda \quad (5)$$

and compared with the standard values. The lattice parameter, a, for ZnTe cubic phase structure was determined by the relationship:

$$a = d_{hkl}\left(h^2 + k^2 + l^2\right)^{1/2} \quad (6)$$

Fig. 5 shows that the film crystallites are prefer oriented with (111) planes, in addition to other reflections (222), (220) , the average cubic lattice parameters ranged between6.140 ± 0.005 and 6.081 ± 0.005 as substrate temperature changed from 298 to 510 K as shown in table 1. By increasing the substrate temperature, a significant increase of peak intensities planes takes place. The high degree orientation is observed for film at substrate temperature of 510 K. This behavior is due to tellurium excess atoms in the films. These atoms may diffuse at crystallite boundaries and form Te microcrystalline.

Table 1: The values of the inter planar spacing and cubic lattice Parameters of ZnTe thin films for different substrate temperatures

T_S [K]	$d\,[\overset{0}{A}]$	Average $a\,[\overset{0}{A}]$	(hkl)
298	**3.558**	**6.140**	**(111)**
	1.767		**(222)**
410	**3.556**	**6.081**	**(111)**
	2.164		**(220)**
	1. 841		**(311)**
	1.767		**(222)**
	1.600		**(331)**
510	**3.555**	**6.078**	**(111)**
	2.163		**(220)**
	1.841		**(311)**
	1.767		**(222)**
	1.598		**(331)**

The crystallite size, D, was determined using the Debye–Scherrer formula [8,28]

$$D = k\,\lambda\left(\beta_{2\theta}\cos\theta\right)^{-1} \quad (7)$$

where, k is the Scherrer constant (k = 0.90), k denotes the wavelength of used radiation (for $\lambda_{CoK\alpha}$ = 1.789 $\overset{0}{A}$) and $\beta_{2\theta}$ is the full width at half-maximum of the peak considered. The crystallite size(ranged between 26.29 and 43.35 nm), increases with increasing substrate temperature from 298 to 510 K. After heat treatment, the films show an enlargement of the large crystallites and the structure is also strongly densified.

Conclusion:

- The method used here was useful to determine the transition types in the ZnTe thin films, which is studied in this experiment.
- Optical study of the our samples indicates the presence of indirectly allowed transition.
- The optical gap E_g decreases after heating substrate of the investigated films, this may be due to the increase in the number of surface dangling bonds.

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بعض الخواص البصرية لأغشية (ZnTe)

الرقيقة المحضرة بتقنية التبخير الحراري على قواعد زجاجية

عبدالله سعيد با صبيح محمد علي صيام

الملخص

تم تحضير أغشية رقيقة من ZnTe بتقنية التبخير الحراري على قواعد زجاجية عند درجات حرارة ترسيب مختلفة ، كما تم تحليل نتائج القياسات البصرية باستخدام برنامج حاسوبي لأجراء التفاضل العددي لنتائج القياسات البصرية، وقد أوضحت هذه التحليلات أن ميكانيكية الانتقال الالكتروني في العينات التي المدروسة من نوع الانتقال غير المباشر المسموح ، وقد تم حساب فجوة الطاقة البصرية ، حيث أوضحت هذه الحسابات نقصان فجوة الطاقة البصرية من 1.15 إلى 0.96 eV عند زيادة درجة حرارة الترسيب من 410 إلى 510, K حيث تم تفسير هذه النتائج باعتبار زيادة التبلور وتشبع العيوب التي تم التحقق منها بأجراء فحوصات حيود الأشعة السينية.

الكلمات المفتاحية: أغشية تولريد الزنك الرقيقة ، فجوة الطاقة البصرية، الانتقالات الالكترونية.