



The effect of substrate temperature on the structural, optical and electrical properties of vacuum deposited ZnTe thin films

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ABSTRACT

The present paper reports the effect of substrate temperature on the structural, optical and electrical properties of vacuum deposited zinc telluride (ZnTe) thin films. X-ray diffraction (XRD) analysis of the films, deposited on glass substrates, revealed that they have cubic structure with strong (111) texture. Room temperature deposits are tellurium rich and an increase in the substrate temperature up to 553 °K results in stoichiometric films. Electrical conductivity has been observed to increase with the increase in substrate temperature, accompanied by increase in the carrier concentration and the mobility of the carriers. The optical bandgap energy and the thermal activation energy of the films have also been evaluated.

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1. Introduction

The II–VI compound semiconductors have attracted many researchers, over the years, because of their possible applications in the fabrication of solar cells, light emitting diodes, photo diodes, photo detectors and many other opto-electronic devices. Zinc Telluride (ZnTe) is one of the important members of the II–VI group, having electrical and optical properties suitable for the fabrication of various opto-electronic devices. It has a wide and direct bandgap of 2.26 eV (at room temperature) [1,2] which is in the pure green region of the electromagnetic spectra. This direct bandgap of 2.26 eV makes it a potential candidate for the fabrication of pure green LEDs [3–6]. Because of its high electro-optic coefficient, ZnTe also promises to be useful in the production and detection of terahertz (THz) radiation [3,7]. Since there is only a small valence band offset of 0.1 eV between ZnTe and CdTe, ZnTe can be used as a back contact material to obtain higher efficiency in CdTe based solar cells [8].

Though some research groups have reported the fabrication of ZnTe based devices like LEDs and terahertz detectors, most of them have preferred higher-end methods like molecular beam epitaxy (MBE), metal organic chemical vapor deposition (MOCVD), etc. to obtain ZnTe films [3–8]. However, vacuum deposition technique, which is simple and economical compared to MBE and MOCVD

techniques, may also yield device quality ZnTe films if the deposition conditions are properly optimized. Substrate temperature is one of the key deposition parameters in the vacuum deposition technique. It influences the composition and crystallinity of the deposited films, and offers a wide range of possibilities. Hence the investigation of the effect of substrate temperature on the properties of vacuum deposited thin films is of great importance. In the present paper an attempt has been made to study the effect of substrate temperature on the structural, optical and electrical properties of vacuum deposited ZnTe films.

2. Experimental details

ZnTe films were deposited on well-cleaned glass substrates by thermally evaporating 99.99% pure ZnTe ingots (from Aldrich) in a molybdenum boat, inside a 12-inch vacuum chamber (HINDHI-VAC 12A4D). A pressure of about 10^{-5} Pa was maintained within the vacuum chamber at the time of deposition. The glass substrates were kept at various temperatures ranging from 300 ° to 553 °. The deposition rate was maintained at, about, 30 nm/min. The films obtained were uniform and had good adhesion to the substrate. Typical ZnTe films having thickness ranging from 300 nm to 900 nm, deposited at various substrate temperatures, were used for characterizations. The X-ray diffraction (XRD) studies of the films were performed by Rigaku Miniflex X-ray diffractometer (CuK α radiation). JEOL (JSM 5800) EDAX unit was used for the compositional studies of the films. The optical bandgap of the films was

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determined by a UV–Visible spectrophotometer (Ocean Optics). For the electrical characterization silver contacts were made on the films by vacuum deposition. Silver was found to form good ohmic contacts with the ZnTe films. The current and voltage measurements were made by Keithley Source Meter (Model 2400) and Multimeter (Model 2002). The variation of resistance of the films with ambient temperature was studied by heating the films in a hot air oven. In order to obtain reliable and accurate values, the readings were taken only during the third cooling period. Hall effect measurements were made for the films by Van-der-Paw method [9].

3. Results and discussion

3.1. Structure and composition

The XRD patterns of the films deposited at various substrate temperatures are shown in Fig. 1. The films have cubic structure with highly preferred orientation in (111) direction. The lattice constant 'a' for (111) planes was found to be about 6.108 Å which is very close to the standard value mentioned in JCPDS (15-0746) data cards. The grain sizes of the films calculated from these XRD patterns are given in Table 1. The increase in grain size, or in other words, the improvement in crystallinity of the films deposited at elevated substrate temperature is due to the greater mobility of the atoms on the heated substrates which in turn results in lesser number of nucleation centers [10].

The chemical composition of the films deposited at different substrate temperatures, is given in Table 2. The films deposited at room temperature are rich in tellurium. As the substrate temperature increases, the Zn:Te atomic ratio increases and approaches unity. Like many other II–VI compounds, ZnTe also undergoes dissociation during thermal evaporation [11]. The zinc and tellurium have different vapor pressures and undergo evaporation to different extents. Hence the resultant vapor itself will be non-stoichiometric. The composition of the film depends on how many zinc and tellurium atoms (or molecules) impinge on the substrate and also on what percentage of these atoms (or molecules) successfully adsorb to the surface of the substrate (i.e. on the sticking coefficient of the impinging atoms or molecules). Thus the

excess of tellurium in the films, deposited at lower substrate temperatures, is due to the difference in vapor pressures and sticking coefficients of zinc and tellurium. When the substrate is heated, the excess tellurium re-evaporates and also the sticking coefficient of zinc increases leading to a balance between zinc and tellurium.

3.2. Optical properties

Fig. 2 shows the absorption spectra of ZnTe films deposited at various substrate temperatures. The absorption coefficient, ' α ' is related to the optical bandgap E_g by the relation [12],

$$\alpha h\nu = B(h\nu - E_g)^n \quad (1)$$

where h is Planck's constant, ν is the frequency of the radiation, B is a constant which depends on the nature of transition and n is a number which can take the values 1/2, 3/2, 2 or more depending on whether the transition is direct-allowed, direct-forbidden, indirect-allowed or indirect-forbidden. In the present case of ZnTe thin films, the plots of $(\alpha h\nu)^2$ vs. $h\nu$ (Fig. 3) show a linear portion indicating that the relation in Eq. (1) holds good for ZnTe films if $n = 1/2$. This means that the optical transitions in the case of ZnTe films are direct transitions. The linear portions of the curves were extrapolated to get the optical bandgap (Fig. 3). The optical bandgap decreases with substrate temperature and approaches the bulk value of 2.26 eV. The shift in the optical bandgap can be attributed to the improvement in crystallinity and the stoichiometry of the films deposited at elevated substrate temperature [11]. Since the films deposited at higher substrate temperatures have large grain sizes and are nearly stoichiometric their optical bandgap is very close to that of the bulk material.

3.3. Electrical properties

Conventional hot probe technique was used to determine the majority carrier type in the ZnTe films, deposited at various substrate temperatures and it was found that all the films were of p-type. This result was later confirmed by Hall effect measurements. In the case of films deposited at relatively lower substrate temperatures, excess of tellurium is responsible for the films to

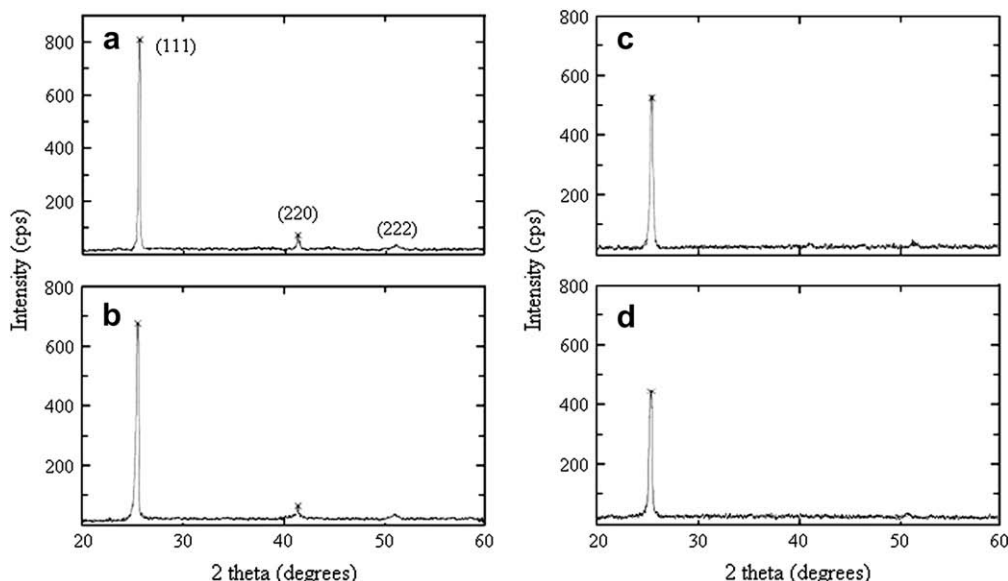


Fig. 1. XRD patterns of ZnTe films deposited on the substrates kept at (a) 553 °K, (b) 473 °K, (c) 373 °K and (d) 300 °K, respectively.

Table 1

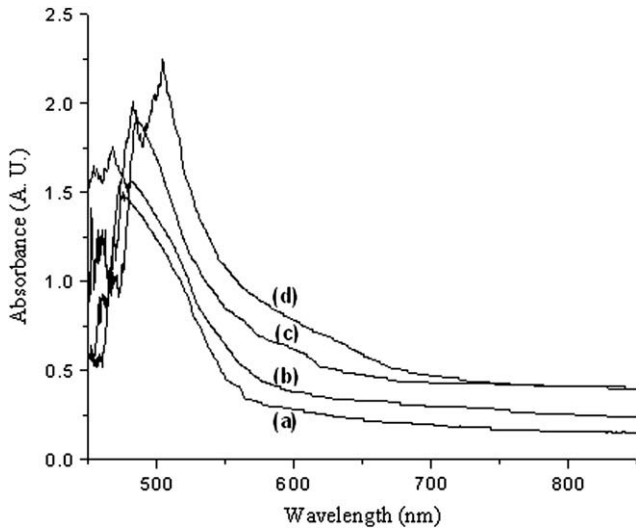
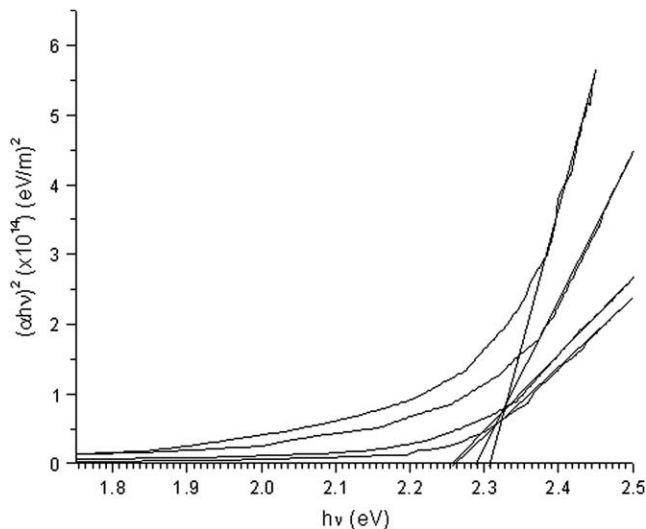
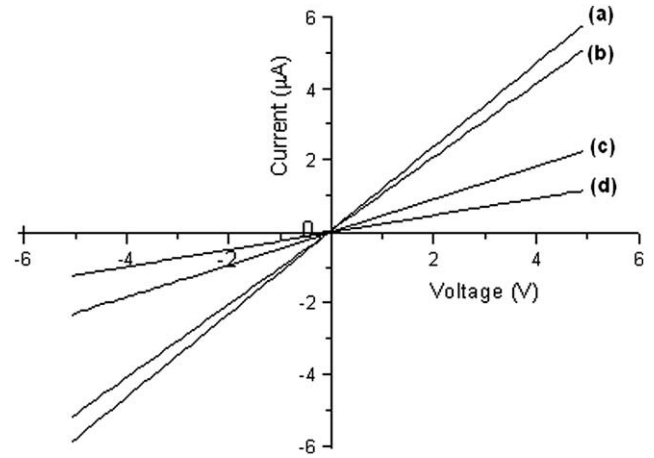
Grain size of the films deposited at different substrate temperatures.

Substrate temperature (°K)	Grain size D (Å)
553	552
473	503
373	433
300	379

Table 2

Zn:Te atomic ratio for films deposited at different substrate temperatures.

Substrate temperature (°K)	Zn:Te
553	1.01
523	0.97
473	0.94
373	0.88
300	0.84

**Fig. 2.** The absorption spectra of the films deposited on the substrates kept at (a) 553 °K, (b) 473 °K, (c) 373 °K and (d) 300 °K, respectively.**Fig. 3.** The $(\alpha hv)^2$ vs. hv plots for films deposited on the substrates kept at (a) 553 °K, (b) 473 °K, (c) 373 °K and (d) 300 °K, respectively.**Fig. 4.** The I - V characteristics of the films deposited on the substrates kept at (a) 553 °K, (b) 473 °K, (c) 373 °K and (d) 300 °K, respectively.

become p-type. However, even the films deposited at higher substrate temperature, which are nearly stoichiometric, were found to be p-type. This may be due to the self-compensation effect which has been observed in ZnTe and other II–VI compound semiconductor films [13]. The I - V plots of the films deposited at different substrate temperatures are shown in Fig. 4. These plots indicate ohmic conduction. The Hall effect measurements were carried out on these films using Van-der-Paw setup. The carrier density, carrier mobility and resistivity of the films obtained from Hall effect measurements are given in Table 3. It was found that the electrical resistivity of the films decreases with substrate temperature. This decrease in the resistivity can be seen as a consequence of improved crystallinity and stoichiometry of the films deposited at higher substrate temperatures. The films deposited at lower substrate temperatures have very small grain size and large grain boundary region. This grain boundary region is highly disordered; having large number of defect states due to incomplete atomic bonding or lack of stoichiometry. These states known as trap states act as effective carrier traps, impeding the flow of majority charge carriers between the grains [14]. The films deposited at higher temperatures are nearly stoichiometric and have larger grains. This would result in a decrease in the defect states and hence an increase in the conductivity of the films.

The variation of electrical resistance, ' R ', of the films with ambient temperature, ' T ', was studied for films deposited at different substrate temperatures in order to understand the conduction mechanism in the films. The plots of $\log R$ vs. $1/T$ were drawn as shown in Fig. 5. All these plots show two different types of conduction regions; namely impurity conduction region, at relatively lower temperatures, and intrinsic conduction region, at higher temperatures. In both the regions, resistance decreases with temperature indicating that the films are semiconducting in nature. The bandgap and thermal activation energy of the films were determined from these plots and the values are given in Table 4. A

Table 3

Electrical parameters of the films deposited at different substrate temperatures.

Substrate temperature (°K)	Carrier density ($\times 10^{20} \text{ m}^{-3}$)	Resistivity (Ωm)	Mobility ($\times 10^{-3} \text{ m}^2 \text{ V}^{-1} \text{ s}^{-1}$)
553	5.79	2.87	3.76
473	5.46	3.10	3.69
373	4.16	7.09	2.12
300	3.17	15.38	1.28

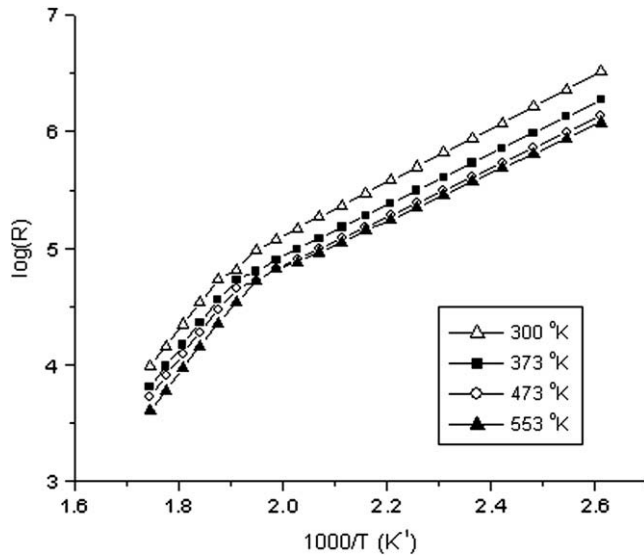


Fig. 5. $\log(R)$ vs. $1/T$ plots of films deposited at different substrate temperatures.

Table 4

The electrical bandgap and thermal activation energies of the films deposited at different substrate temperatures.

Substrate temperature (°K)	Bandgap (eV)	Thermal activation energy (eV)
553	2.27	0.81
473	2.27	0.83
373	2.27	0.87
300	2.28	0.91

very small change in the thermal activation energy and bandgap is observed with the increase in substrate temperature. Since all the films were heated to a high temperature, thrice before taking the readings, the films might have undergone some annealing. Therefore it is hard to determine the degree of dependence of the bandgap and thermal activation energy on the substrate temperature.

4. Conclusions

Vacuum deposition technique was employed to deposit ZnTe thin films on glass substrates and the substrate temperature was used as a tool for tailoring the structural optical and electrical properties of the films. The films deposited at higher substrate temperatures were found to have larger grains and nearly stoichiometric composition. These improvements in grain size and composition were further found to enhance the optical and electrical properties of the films. Thus both good crystallinity and stoichiometric composition, which are the prerequisites for device quality films, can be achieved in vacuum deposited ZnTe films by suitably varying the substrate temperature.

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