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Nanocrystalline Zn_xTe_{100-x} (x = 0, 5, 20, 30, 40, 50) thin films: Structural, optical and electrical properties



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ABSTRACT

In the present paper, the structural, optical and electrical properties of nanocrystalline Zn_xTe_{100-x} (x=0,5,20,30,40,50) thin films (average thickness ~ 350 nm), deposited by thermal evaporation, have been studied. The X-ray diffraction results revealed that single phase Zn_xTe_{100-x} was obtained at x=50. Fourier transform infrared spectra also revealed the formation of zinc blende phase at x=50. Energy dispersive X-ray spectroscopy confirms the elemental composition. Field emission scanning electron micrographs confirmed the uniform deposition of all thin films. UV–Vis–NIR results revealed that the optical band gap, calculated by Tauc's plots, increases with increase in Zn content. This may be due to the alloying effect. Temperature dependent dark conductivity showed that conductivity is thermally activated process having single activation energy in the measured temperature range (300–375 K). The dark conductivity and activation energy decreased with increase in Zn content. The explanations of variation in the properties of ZnTe with increase in Zn percentage have been provided.

1. Introduction

In recent years, II-VI group chalcogenide materials have attracted great attention of scientists around the globe because of their wide range applications as solid-state devices both in technological and scientific field [1]. Moreover, these materials are economically viable for the production of low cost photovoltaic devices [2]. This group semiconductors (such as ZnO, ZnS, ZnSe, ZnTe, CdO, CdS, CdSe, and CdTe) have direct and wide band gap due to which these are widely used in the fabrication of solar cells and optoelectronic devices [3,4]. Among them ZnTe is one of the exciting semiconductor material with optimum band gap (~ 2.26 eV at room temperature) [5] and low electron affinity (3.53 eV) [6]. It is usually a p-type semiconductor [7] with cubic [8] or hexagonal structure that depends upon the synthesis conditions [9]. Such parameters make it useful in design of green LEDs [10], IR detectors [11], high efficient powder-phosphor screens [12], THz emitters [13], detectors [14], opto-refractive materials for non-polarized memory switching and optical data processing ray detectors [15,16]. ZnTe is also used as a back contact layer in CdTe based solar cells. It provides higher efficiency in these solar cells due to small valence band offset of 0.1 eV between ZnTe and CdTe [17]. These applications are closely related to variation in optical and structural properties of ZnTe thin films [6].

To the present, various methods such as, RF sputtering [18], electro deposition [19], thermal evaporation [20], DC sputtering [21], vapour phase epitaxy [22], closed space sublimation [23], molecular beam epitaxy [24], magnetron sputtering [25], electrochemical process [26], metal organic vapour phase epitaxy (MOVPE) and metal organic chemical vapour deposition (MOCVD) [27] have been used to synthesize ZnTe thin films. Among these methods, thermal evaporation technique provides thin films on large area and gives better control of deposition rate, film thickness and temperature [28].

Various research groups [29–32] have reported the study on optical, structural and electrical properties of ZnTe thin films. However, the compositional dependent study on structural, optical and electrical properties of ZnTe thin films has been limitedly reported. Kishore et al. [33] has studied the structural and thermal transport properties of ${\rm Zn_xTe_{100-x}}$ (x=5,10,30 and 50) alloys in pellet form. They reported that the diffraction results of ${\rm Zn_50Te_{50}}$ composition show the presence of both Te and ZnTe phases. Sharma et al. [34] prepared the ${\rm Zn_xTe_{100-x}}$ (x=5,10,30 and 50) pellets of 99.99% purity and reported the XRD result for ${\rm Zn_5Te_{95}}$. Hexagonal Te exhibits most diffraction peaks as compare to cubic ZnTe. The workers used reflection spectroscopic technique to investigate the optical properties of these pellets. They

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found excellent agreement in the optical band gap of laboratory prepared $Zn_{50}Te_{50}$ and commercially obtained pure $Zn_{50}Te_{50}$.

In the present study, effort has been made to investigate the effect on structural, optical and electrical properties of pure Te after Zn incorporation in five different compositions $(Zn_xTe_{100-x}; x=5, 20, 30, 40, 50)$. This study is useful in providing the knowledge of structural, optical and electrical properties of ZnTe at different Zn/Te compositions which is essential in fabrication of opto-electronic devices.

2. Experimental details

Zinc and tellurium (99.999% pure) were procured from Sigma-Aldrich, India, $Zn_x Te_{100-x}$ (x = 0, 5, 20, 30, 40, 50) allows with different compositions were prepared by conventional melt quenching technique [35]. Thin films from these alloys were deposited on welldegassed glass substrates by thermal evaporation technique using Hind HIVAC system (Model: BC-300) in a vacuum of $\sim 4 \times 10^{-6}$ mbar. Deposition was performed at slow deposition rate of 2-3 Å/s to make the composition of thin films close to starting bulk material. The thickness of thin films was monitored in situ using digital thickness monitor (DTM-101) and calculated using cross-sectional FE-SEM. The average thickness of the films was estimated to be $\sim\,350\,\text{nm}.$ The structural study was performed using PANalytical X'pert PRO X-ray diffractometer with CuK_{α} radiation ($\lambda = 1.54060 \text{ Å}$) over the range of $20^{\circ} \le 2\theta \le 70^{\circ}$. For morphological study, Field emission scanning electron microscope (FE-SEM) results were obtained using Hitachi-SU8010 and the composition of films was estimated using Energy-dispersive spectroscopy (EDS) with the help of Bruker X-flash, 6130. For optical studies, Fourier transform infrared (FT-IR) spectrum has been recorded using BRUKER-ALPHA in spectral range of 4000-600 cm⁻¹. A double beam UV-Vis-NIR spectrophotometer (Perkin Elmer Lambda 750) was used in the transmission range 300-2700 nm, to measure normal incidence transmission spectra of thin films. All the optical constant measurements reported in this paper were performed at room temperature (300 K). A specially designed metallic sample holder was used for electrical measurement of all ZnTe thin films in a planar geometry (electrode gap $\sim 8 \times 10^{-2}$ cm). The electrical conductivity was measured using a two-probe method and for Ohmic electrical contacts, thick indium electrodes were pre-deposited by thermal evaporation at room temperature. A vacuum of $\sim 10^{-3}$ mbar was maintained throughout the electrical measurements using rotary pump (MAC: OFVP-25A). A constant voltage power supply (Model: EHT-11) and a digital multimeter (MARS: VC890-D) were used to record the conductivity in these films. The temperature of film was controlled by specially designed heater and was measured by a chromel-alumel thermocouple placed on the substrate [36]. The Hall measurements were performed using the van der Pauw configuration on samples with area of $4 \times 4 \text{ mm}^2$. Thin films were mounted on an insulated holder and a magnetic field of 3.0 kG was applied. Four silver contacts (size ~ 1 mm²) were deposited on the corners of the samples, taking care that

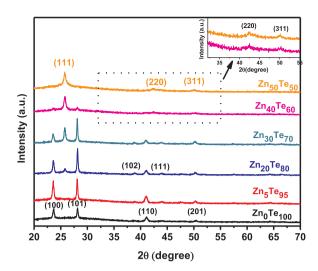
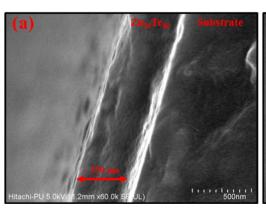


Fig. 2. X-ray diffraction patterns for all $Zn_xTe_{100\,-\,x}$ thin films.

the contact size was always much smaller than the distance between the contacts.

3. Results and discussion

Fig. 1(a, b) presents the cross sectional FE-SEM images of Zn₃₀Te₇₀ and Zn₅₀Te₅₀ thin films. The average thickness of all the films were found to be ~ 350 nm. The X-ray diffraction (XRD) results for Zn_xTe_{100-x} (x = 0, 5, 20, 30, 40, 50) thin films are represented in Fig. 2. Comparison of XRD pattern of elemental Te with standard data reveals hexagonal crystal structure with diffraction peaks at 2θ equals to 23.67°, 28.15°, 38.70°, 41.12°, 43.75° and 50.37° corresponding to (100), (101), (102), (110), (111) and (201) orientations [ICDD Card no. 00-003-0506]. Comparing other films with standard reveals that, with increase in Zn composition, there is the emergence of cubic ZnTe phase along with hexagonal phase of Te. More specifically, ZnTe phase starts emerging around $2\theta = 25.81^{\circ}$ for x = 20 thin film. The intensity of this peak goes on increasing, as the composition of Zn further increases up to x = 50. Conversely, the decrease in intensity of Te peaks (hexagonal phase) along (100) and (101) orientations is observed (Fig. 2). Finally for x = 50, all the peaks corresponding to hexagonal Te phase diminished and single phase ZnTe with cubic crystal structure is obtained with diffraction peaks at 2θ equals to 25.77°, 42.38° and 50.07° corresponding to (111), (220) and (311) orientations [ICDD Card no. 01-079-004]. The position of XRD peaks has been shifted towards lower angles (2θ) with increasing concentration of Zn, which might be due to expansion of lattice parameters [37]. The crystallite size was calculated by Scherrer formula [38]:



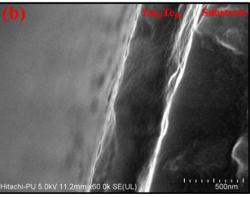


Fig. 1. Cross-sectional FE-SEM images for (a) $Zn_{20}Te_{80}$ and (b) $Zn_{50}Te_{50}$ thin films.

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