

Effect of Substrate Temperature on Structural and Optical Properties of Nanocrystalline CdTe Thin Films Deposited by Electron Beam Evaporation

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Nanocrystalline Cadmium Telluride (CdTe) thin films were deposited onto glass substrates using electron beam evaporation technique. The effect of substrate temperature on the structural, morphological and optical properties of CdTe thin films has been investigated. All the CdTe films exhibited zinc blende structure with (111) preferential orientation. The crystallite size of the films increased from 35 nm to 116 nm with the increase of substrate temperature and the band gap of the films decreased from 2.87 eV to 2.05 eV with the increase of the crystallite size.

Keywords: CdTe thin films, Electron beam evaporation, Structural properties, Optical properties.

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1. INTRODUCTION

II-VI compound semiconducting thin films have drawn considerable interest for the past two decades as they find enormous applications in fabrication of photoconductors, space charge limited diodes, photovoltaic cell, transistors and infra-red (IR) detectors [1]. Among the various II-VI compound semiconductors, CdTe with a narrow direct band gap of 1.45 eV and high absorption coefficient ($\alpha > 10^4 \text{ cm}^{-1}$) is one of the promising candidates for IR detector, photovoltaic, optoelectronic applications. In addition, CdTe is low cost and most stable absorber material for processing of solar cell with good efficiency. Several deposition methods such as close spaced sublimation [2-3], electro deposition [4], sputtering [5] close spaced vapor transport [6], spray pyrolysis [7], metal organic chemical vapor deposition [8-9] and vacuum evaporation [10] were employed for the deposition of CdTe thin films. Among these methods, electron beam evaporation is more advantage because of avoiding impurities during film growth, the tendency to form oxides can be considerably reduced and very slow rate of deposition [11-12] is possible. The structural and optical properties of the films generally depend on the deposition conditions such as rate of evaporation, substrate temperature and the film thickness. Hence optimization of the deposition conditions is very important to get good quality thin films. In the present study, an attempt is made to prepare nanocrystalline CdTe thin films by electron beam evaporation and to study the effect of substrate temperature on structural and optical properties of the CdTe thin films.

2. EXPERIMENTAL DETAILS

2.1 Deposition of CdTe films

CdTe (4N pure, M/S Sigma Aldrich) in the form of powder was taken as a source material and loaded into the graphite crucible. Corning 7059 glass slides were cleaned in ultrasonic bath with acetone and then washed with distilled water for 10 min. After that the substrates were dried in hot air oven and fixed to the substrate

holder. CdTe thin films were deposited using electron beam evaporation (Hind High Vac Model: 12A4D). The metal chamber was then evacuated to a pressure of about 1×10^{-6} mbar. CdTe films were coated onto the glass substrates at different substrate temperatures ($T_s = 423 \text{ K}$, 573 K , 623 K and 673 K) with a slow rate of deposition $6\text{-}8 \text{ \AA/s}$. A distance of 10 cm was maintained between the source and the substrate. Thickness of the films was controlled using quartz crystal thickness monitor (QTM). The thickness of the samples deposited at different substrate temperatures was about 400 nm.

2.2 Characterization of Techniques

The crystallographic structure of the films were examined by X-ray diffractometer (XRD) (Bruker D-8 Advance) using the monochromatic $\text{CuK}\alpha$ radiation ($\lambda = 1.5406 \text{ \AA}$). The surface morphology and elemental composition analysis of the films were studied using High Resolution scanning electron microscope (FEI Quanta FEG-200) coupled with energy dispersive analysis of X-rays (EDAX). The optical transmittance of the films was recorded using UV-Vis-NIR double beam spectrophotometer (JASCO-V-670) in the wavelength range 200-2500 nm.

3. RESULTS AND DISCUSSIONS

3.1 Structural Properties

The X-ray diffraction patterns of CdTe thin films deposited at 423 K, 573 K, 623 K and 673 K substrate temperatures are shown in Fig. 1. XRD patterns confirm that the films are poly crystalline in nature and the major diffraction peak was oriented along (111) plane which reflects the zinc blende structure of the CdTe thin films. The films formed at 573 K exhibited (222) and (311) orientations at diffraction angles 39.30° and 46.43° , respectively. The intensity of films remained same up to 573 K and it increased when the substrate temperature of the films increased from 573 K to 673 K which may be due to increase in the grain size of the deposited films.

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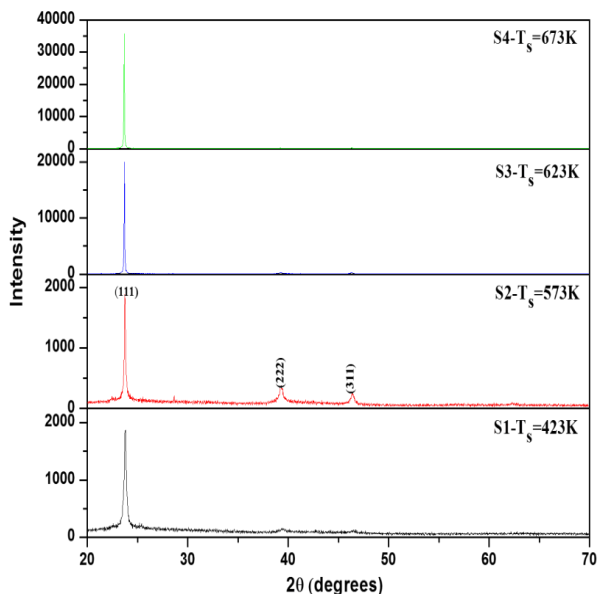


Fig. 1 – X-ray diffraction patterns of the CdTe thin films deposited at 423 K, 573 K, 623 K and 673 K

Fig. 2 shows the variation of lattice constant and micro strain of CdTe thin films with substrate temperatures from 423 K to 673 K. The lattice parameter has been calculated from the predominant peak (111) and it varies linearly with the increase of substrate temperature, whereas the micro strain decreased with the increase of substrate temperature. The lattice parameter of the films increased from 6.47 Å to 6.50 Å when the substrate temperature of the films increased from

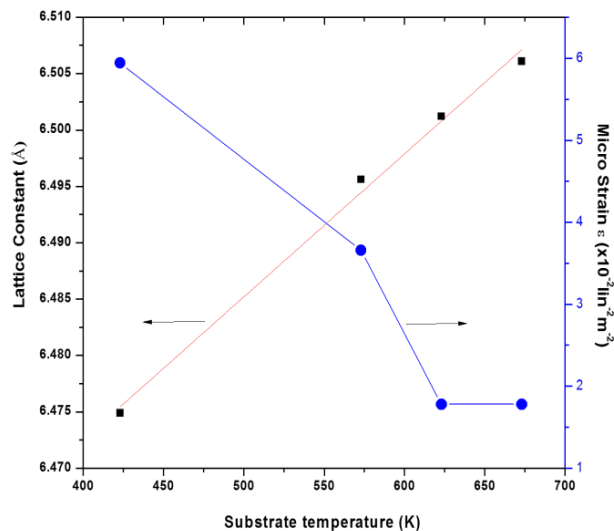


Fig. 2 – Variation of lattice parameter and microstrain with increase of substrate temperature

Table 1 – Summary of crystallite size, lattice constant, microstrain and band gap of the films deposited at different substrate temperatures

Film Name	T_s (K)	2θ (degree)	FWHM	Lattice constant a (Å)	Crystallite Size D (nm) XRD	Crystallite Size D (nm) SEM	Micro strain	Band gap (eV)
S1	423	23.78	0.243	6.475	35	31	5.94	2.87
S2	573	23.76	0.150	6.496	57	70	3.66	2.47
S3	623	23.68	0.088	6.501	96	–	1.78	2.07
S4	673	23.66	0.073	6.506	116	108	1.78	2.05

423-673 K. The increase in the lattice constant with the increase of substrate temperature may be due to internal stress developed in the film grains, which triggers the prolongation. The decrease in microstrain with the increase of substrate temperature may be due to the difference in the temperature coefficient of expansion of the glass substrate and CdTe thin films. The grain size of the films has been calculated using Debye Scherrer formula. The grain size increases from 35 nm to 116 nm with the increase of substrate temperature. As the substrate temperature increases the adatom mobility also increases and the FWHM decrease and resulted increase in crystallite size [13]. Similar kind of behavior was observed in CdTe thin films prepared by other preparation methods [14-18]. A summary of crystallite size, lattice constant and microstrain and band gap of the films deposited at different substrate temperatures is given in Table 1.

3.2 Morphological and Composition Analysis

Fig. 3 shows the high resolution scanning electron microscope (HRSEM) images of the CdTe thin films deposited at different T_s . From the HRSEM images, film surface seems to be regular and the grain size increased with substrate temperature [19]. The observed grain size from SEM is almost equal to that calculated from XRD data. Fig. 4 shows typical EDAX spectrum of the CdTe thin film deposited at 573 K. From EDAX analysis, it was found that all the films were nearly stoichiometric. But the small difference between Cd (46.26 at. %) and Te (53.8 at. %) atomic percentage is due to the high vapor pressure of Te when compared to that of Cd.

3.3 Optical Properties

Fig. 5 shows the optical transmittance spectra of the CdTe thin films deposited at different substrate temperatures. All the films exhibited poor optical transmittance in the visible region. From the transmittance spectra it was clear that the absorption edge of the films moved towards the higher wavelengths with increase in substrate temperature. The optical band gap of the films was calculated using the Tauc's relation [20],

$$\alpha h\nu = A(h\nu - E_g)^r \tag{3.1}$$

where A is a constant which is different for different transitions indicated by different values of r , h is the Planck's constant, ν the frequency of light, E_g the optical band gap and ' r ' a parameter which characterizes the transition process involved. The parameter r takes the values of 2 and 1/2 for the direct allowed transition and for indirect allowed transition, respectively.

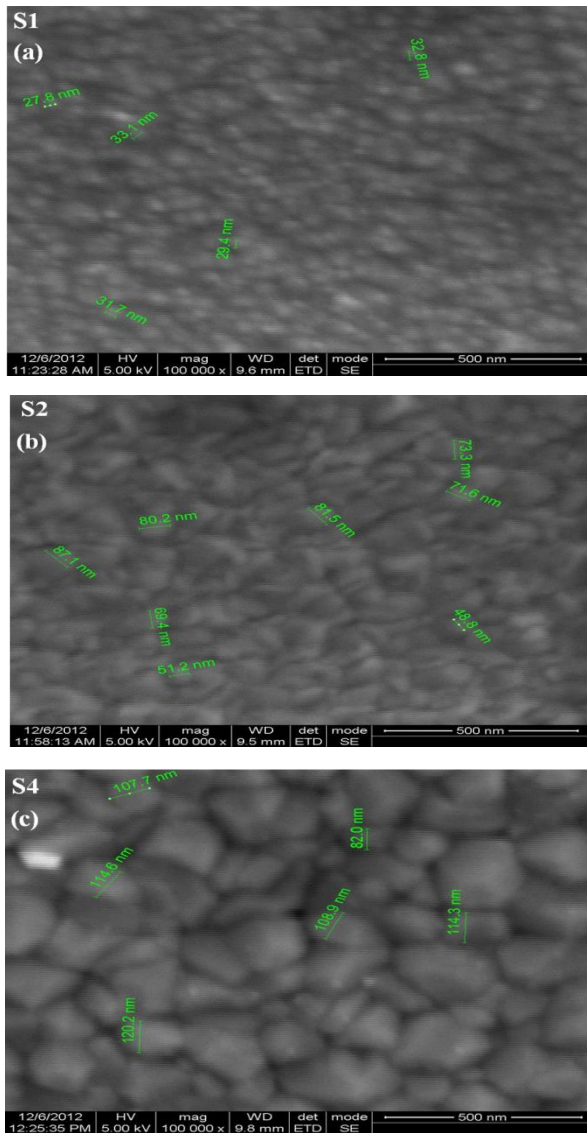


Fig. 3 – HRSEM images of the CdTe thin films deposited at 423 K (a), 573 K (b) and 673 K (c)

From the Fig. 6 it is evident that the optical band gap of the CdTe films decreased with increase of substrate temperature. Similar decrease in band gap with the increase of temperature had been reported in CdTe films deposited by thermal evaporation [21-22]. The CdTe films coated at low substrate temperature (423 K) have an optical band gap of 2.87 eV. Whereas it is 2.05 eV for the film coated at higher substrate temperature (673 K). The actual band gap of the CdTe (bulk) is 1.45 eV. In the present study a clear blue shift was observed in nano crystalline CdTe thin films deposited at different substrate temperatures (T_s) which is obvious due to the quantum confinement.

Fig. 7 shows that as substrate temperature increased the crystallite size increased whereas the band gap decreased. This decrease in band gap may be attributed to an increase in particle size with corresponding increase at substrate temperature.

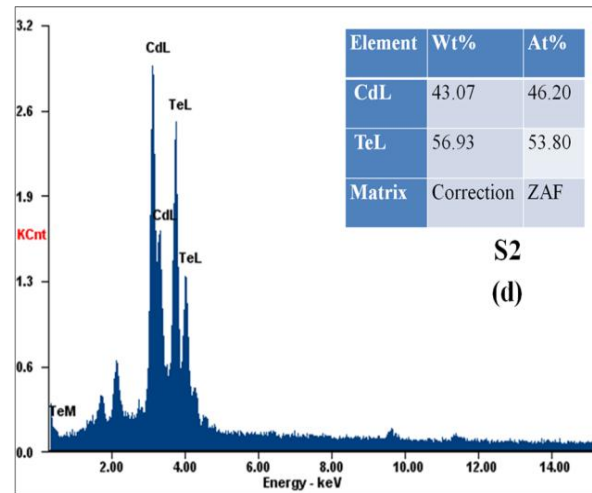


Fig. 4 – Typical EDAX spectrum of the CdTe thin film deposited at 573 K

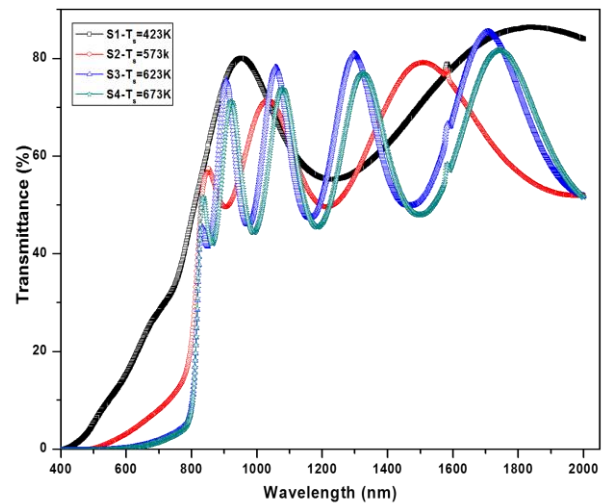


Fig. 5 – Optical transmittance spectra of the CdTe thin films deposited at different substrate temperature T_s

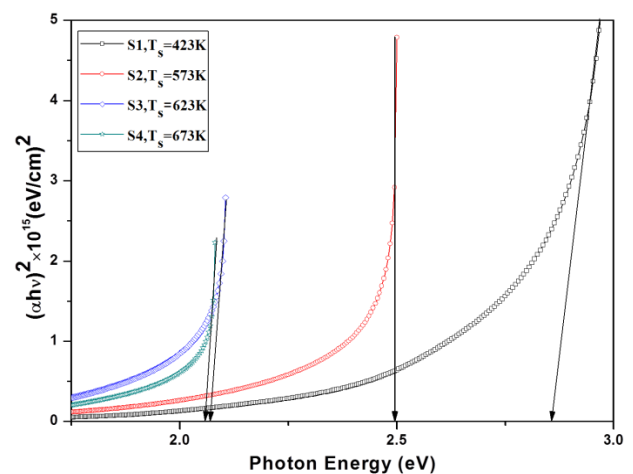


Fig. 6 – Optical band gap plots of CdTe thin films at different substrate temperature T_s

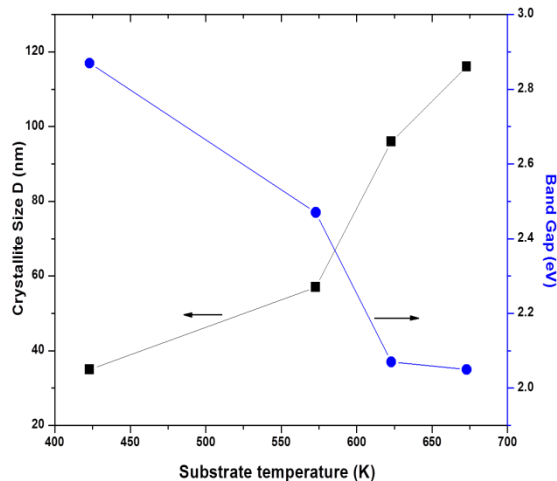


Fig. 7 – Variation of Crystallite Size and Band gap with increase of substrate temperature

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4. CONCLUSION

Nanocrystalline CdTe thin films at different substrate temperatures were deposited by electron beam evaporation technique. The effect of substrate temperature on the structure, morphology and optical properties of the CdTe films was investigated. The structure of the CdTe thin films was zinc blende with a preferential orientation of (111) plane. Morphological studies revealed an increase in the crystallite size with the increase in substrate temperature from 423 K-673 K. The band gap of the CdTe thin films decreased with increase of grain size and substrate temperature.

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