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Effect of Substrate Temperature on the Properties of Nanocrystalline CdTe Thin Films Coated by Electron Beam Evaporation Method

T. Manimozhi[1], K. Ramamurthi[1]*, M. Maria Angelin Sinthiya[1], A. Karthigeyan[1], P. V. Bhuvanaswari[2], R. Ramesh Babu[2]

[1]Crystal Growth and Thin Film Laboratory, Department of Physics and Nanotechnology, SRM University, Kattankulathur 603203, Tamil Nadu, India.
[2]Crystal Growth and Thin Film Laboratory, School of Physics, Bharathidasan University, Thiruchirappalli 620024, Tamil Nadu, India.

Abstract : Nanocrystalline cadmium telluride (CdTe) thin films were deposited by electron beam vacuum evaporation technique on the microscopic glass substrates at different substrate temperatures of 225, 300 and 375˚C. The vacuum pressure was $\sim 1\times10^{-5}$ mbar and the distance between the source and the substrate was 10 cm. The effect of substrate temperature on the structural, morphological and optical properties of nanocrystalline CdTe thin films was investigated. The X-ray diffraction studies showed that the peak intensity increases with increasing substrate temperature. Scanning electron microscopic studies showed uniformly distributed grains on the surface of the film deposited at 375˚C. Elemental analysis of the film showed that the deposited film is rich in Te. The average transmittance of the films in the visible range of the solar spectrum is influenced by the substrate temperature. Photoluminescence spectra of CdTe films, showed a strong emission peak at 560 nm. Fluorescence spectra of CdTe thin films showed the emission peak at 590 nm.
Keywords: CdTe thin films, Nanocrystalline, XRD, SEM, Grain Size, Film Thickness.

Introduction

During the past few decades increasing interest in the preparation and characterization of the metal chalcogenide thin films has emerged, because of their potential applications in solar selective coating, solar control, photoconductor, solid state solar cells, optical imaging, hologram recording and optical mass memories[1]. CdTe belongs to one of the promising II-VI p-type semiconducting chalcogenides and its optical and electrical transport properties make it a potential candidate for the application in many electronic and optoelectronic devices. Theoretical calculation shows that the semiconductors with bandgap energy in the range of 1.00 – 2.00 eV are suitable for efficient solar energy conversion. High absorption coefficient ($>10^4$ cm^{-1}) of CdTe in the visible and near IR region of the solar spectrum and its direct band gap (~1.5 eV) close to the optimum value for efficient solar energy conversion advocate its suitability for solar cell fabrication[2,3]. CdTe thin film based solar cell with an n-type CdS window layer has produced conversion efficiency of about 16%[2].

Further the possibility of alloying the CdTe with other IIB-VIA compounds to alter its band gap and to tune its optoelectronic properties facilitates to design the required optoelectronic devices[4]. Several deposition methods such as thermal evaporation[5-7], electron beam evaporation[8,9], closed space sublimation[10,11], sputtering[12] and spray pyrolysis[13,14] methods were employed to deposit the CdTe thin films. Among these methods, electron beam evaporation has its advantage which avoids the impurities during film growth, considerably reduces the formation of oxides[8] and the slow rate of the deposition creates the possibility to form nanocrystalline CdTe thin films. The nanostructured CdTe thin film exhibits unusual charge carrier dynamics and improves collection of the photogenerated carriers which enhances solar energy conversion efficiency[14]. The structural, electrical and optical properties of the thin films are influenced by the deposition condition such as rate of evaporation, substrate temperature, source to substrate distance and thickness of the films. In the present work nanocrystalline CdTe thin films were prepared by electron beam evaporation method at different substrate temperatures and the effect of substrate temperature on the structural, morphological and optical properties is discussed.

Experimental

CdTe thin films were deposited on the well cleaned microscopic glass substrates by electron beam evaporation method (VR Technologies- Vacuum Coating Unit- Model-VRT-EB GPS-3) at different substrate temperatures (T_s) of 225, 300 and 375˚C. The vacuum pressure was maintained at 1×10^{-5} mbar in the chamber. The distance between the source and the substrate was 10 cm. 0.005g of CdTe powder (Alpha Aesar) was taken in the graphite crucible and evaporated for 5 minutes employing 3 KW EB Gun Power Supply with 20 mA source current.

Results and discussion

Structural Properties

XRD Analysis

CdTe thin films prepared were subjected to X-ray diffraction (XRD) studies using Philips X pert PRO X-ray diffraction system with CuKα radiation of wavelength λ = 1.5406 Å. The X-ray diffraction pattern of CdTe thin films coated at different substrate temperatures is shown in Fig.1. The XRD peaks were compared with JCPDS data[15] (No: 65-1047) which revealed that the peak obtained at the angle (2θ) 44.325˚ represents (220) plane of cubic system of CdTe. The strong XRD peaks at 2θ = 38.04˚ and 2θ = 82.02˚ are due to crystalline Te as evidenced from JCPDS data[16] (No: 65-3370). Intensity of all the XRD peaks increases with increasing substrate temperature, which indicates the improvement on the crystallinility due to recrystallization.

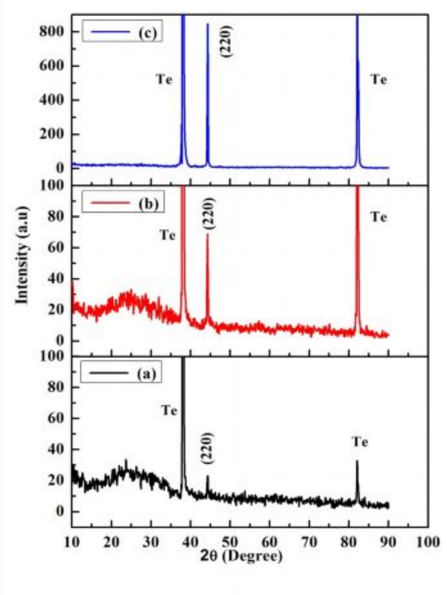


Fig. 1: X – ray diffraction pattern of CdTe thin film deposited at substrate temperature of (a) 225˚C, (b) 300˚C, (c) 375˚C.

The lattice parameter '*a*' of the cubic system of CdTe films prepared at various substrate temperature was evaluated from the relation[17], $a = d\sqrt{(h^2 + k^2 + l^2)}$ where, d is the interplanar spacing and h, k, l are Miller Indies. The crystallite size (D) was determined using Debye Scherrer formula[18], $D = k\lambda/(\beta_{2\theta}\cos\theta)$ where the constant k is the shape factor which is 0.94 for cubic structure, λ is the wavelength of X-rays of CuKα (1.5405Å), θ is the Bragg's angle and $\beta_{2\theta}$ the full width at half maximum (FWHM) of (220) peak in radian. The microstrain (ε) was calculated using the relation[19], $\epsilon = \beta_{2\theta}\cos\theta/4$. Structural parameters of CdTe thin films FWHM, crystallite size and microstrain are calculated and presented along with the film thickness in Table 1. Table 1 shows that the crystallite size increases from ~25 nm to ~37 nm with increase in the substrate temperature from 225˚C to 375˚C and this may be due to improvement of the crystallinity by recrystallization process at 375˚C.

Table 1: Thickness, FWHM, Crystallite Size and Microstrain of CdTe thin films deposited at different substrate temperature.

Substrate Temperature T_s (˚C)	Film thickness t (nm)	FWHM β (Degrees)	Crystallite Size D (nm)	Microstrain (ε)
225	129	0.350	25.61	0.0810
300	300	0.268	33.37	0.0620
375	502	0.240	37.21	0.0555

The thickness of films was estimated by stylus profilometer SJ301 equipment which shows that the thickness of the CdTe films increases with increasing substrate temperature. The microstrain decreases with increase in the substrate temperature, which may be due to the different temperature coefficient of expansion of the glass substrate and CdTe thin films.

Table 2: Comparison of cell parameter and d-spacing value of CdTe thin films deposited at different substrate temperature.

Substrate Temperature T_s (˚C)	2θ (˚)	d- spacing (nm)	Cell parameter (a) (Å)	Reference
225	44.325	0.2043	5.7811	Present work
300	44.325	0.2046	5.7872	Present work
375	44.325	0.2044	5.7815	Present work
JCPDS	44.04	-	5.810	Reference[15]

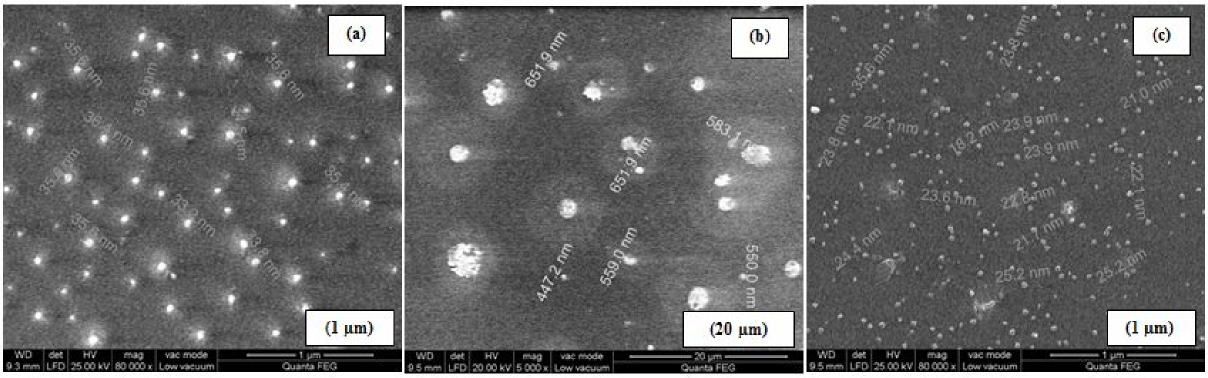
Table 2 shows the d-spacing and cell parameter as a function of substrate temperature calculated from (220) XRD peak of CdTe. The cell parameter calculated compare well with the corresponding value of 5.810 Å (JCPDS No: 65-1047)[15].

Surface Morphological and Composition Analysis

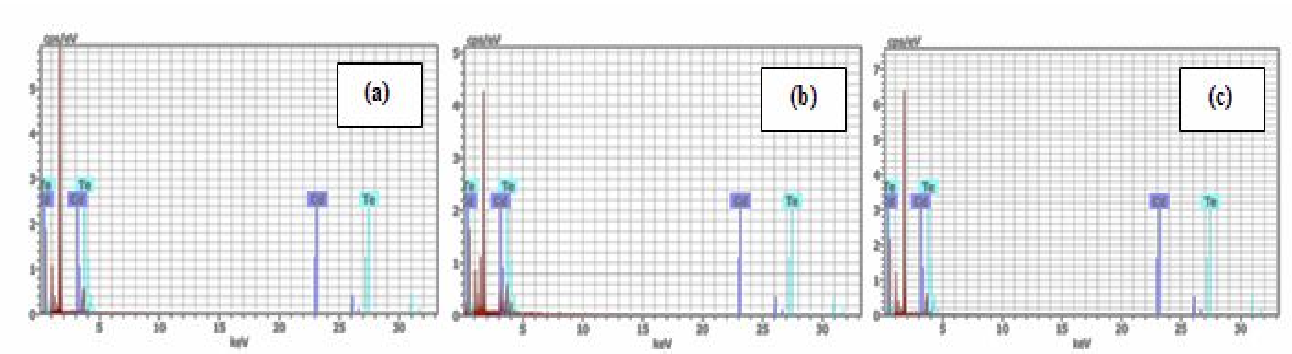
FESEM and EDXS Analysis

Surface morphology and elemental composition of the films were analyzed by the energy dispersive X ray (EDXS) spectrometer interfaced to FEI Quanta 200 FEG scanning electron microscope (FESEM). The field emission scanning electron microscopic (FESEM) images recorded for CdTe films prepared at different substrate temperatures are shown in Figs. 2a-c. FESEM images of the CdTe film show that the surface of the films is uniform and without any observable pinholes or cracks.

Fig. 2a shows that small grains of ~35.13 nm size are spread over the surface of the film deposited at 225˚C. When the substrate temperature was increased to 300˚C, the nanocrystallites form the clusters with various sizes varying from 447 to 652 nm and are distributed on the surface of the film as shown in Fig. 2b. The surface morphology of the CdTe film prepared at the substrate temperature 375˚C is shown in Fig. 2c, which contains nanocrystalline grains of size about 25 nm distributed uniformly over the surface. CdTe thin films prepared on the glass substrates for the deposition period of 1h using RF magnetron sputtering showed that the nanoparticles clustered together to form clusters of about 80 nm[20]. The average grain size in the CdTe film depends upon the substrate temperature and thickness of the film[21].



Figs. 2a-c: FESEM images of CdTe thin film deposited at substrate temperature of (a) 225˚C, (b) 300˚C, (c) 375˚C.



Figs. 3a-c: EDAX images of CdTe film deposited at substrate temperature of (a) 225˚C, (b) 300˚C, (c) 375˚C.

Figs. 3a-c show the typical EDAX spectrum of the CdTe thin films deposited at different substrate temperature. The elemental composition of CdTe thin films deposited at different substrate temperature was estimated by EDAX technique and are presented in Table 3. From the EDAX analysis, it is found that the deposited films contain relatively more concentration of Te due to the high vapour pressure of Te compared to that of Cd at the deposition temperature[8].

Table 3: Elemental composition of CdTe thin films deposited at different substrate temperature.

Substrate Temperature (T_s) (˚C)	Cd		Te	
	at%	wt%	at%	wt%
225	18.91	17.04	81.09	82.96
300	38.76	35.80	61.24	64.20
375	15.33	13.75	84.67	86.25

Optical Properties

UV - vis Spectral Analysis

Fig. 4 shows the optical transmittance spectra recorded for CdTe films prepared at various substrate temperatures using SHIMADZU UV - vis - spectrophotometer in the wavelength range of 190-700 nm.

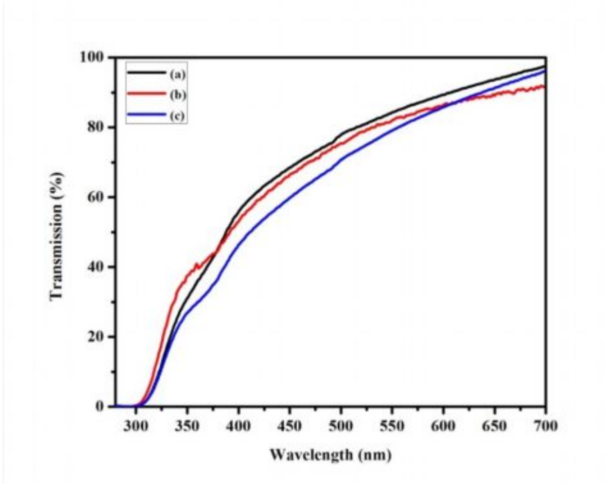


Fig. 4: Transmittance spectra of CdTe film deposited at substrate temperature of (a) 225˚C, (b) 300˚C, (c) 375˚C.

The average transmittance calculated in the visible rang of 400 – 700 nm decreases from 81.8 % (225˚C) to 78.8 % (300˚C) and to 76.4 % (375˚C) with increase in the substrate temperature given in the parenthesis. Further it is also evident that transmittance percentage decreases with the increase in the thickness of the film as a function of substrate temperature (Table 1).

Optical Band gap

The optical band gap (E_g) was calculated using Tauc's relation[22], $\alpha h\nu = A(h\nu - E_g)^n$ where A is a constant, h is the Planck's constant, ν is the frequency of the incident light and n depends upon the nature of band transition. The value of n is ½ for direct allowed transitions. The plots drawn between hν along X-axis and $(\alpha h\nu)^2$ along the Y-axis are shown in Fig. 5.

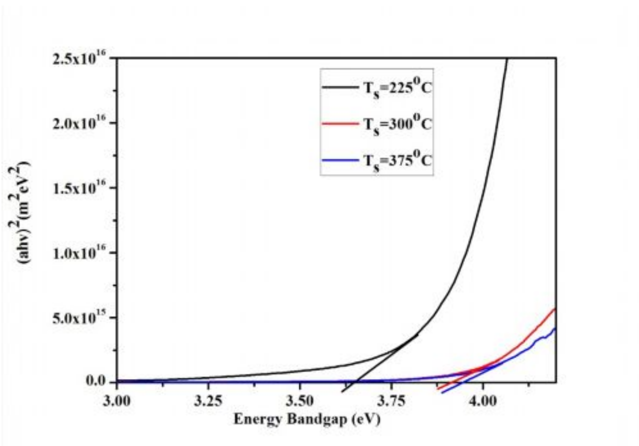


Fig. 5: $(\alpha h\nu)^2$ vs hν plots of CdTe films deposited at substrate temperature of (a) 225˚C, (b) 300˚C, (c) 375˚C.

The direct band gap value of CdTe nanocrystalline films estimated from the extrapolation of linear portion of the curve to zero absorption is 3.64 eV (225˚C), 3.91 eV (300˚C) and 3.94 eV (375˚C) for different substrate temperature given in the parenthesis. Optical band gap of CdTe thin films increases with increase in the substrate temperature. The band gap reported for CdTe film having particle of size of ~10 nm is 2.8 eV as compared to the band gap of 1.5 eV of bulk CdTe[23]. The band gap of nanocrystalline CdTe film prepared at the substrate temperature of 150˚C is about 2.87 eV and the crystallite size of the films is about 31 nm[8]. The band gap value of the present work is compared with the literature values in Table 4. The value of E_g in the present work is relatively large which may be due to increase in the Te content in the coated CdTe film.

Table 4: Comparison of band gap of CdTe thin films deposited at different substrate temperature.

S.No	Substrate Temperature (T_s) (°C)	Thickness of the film (t) (nm)	Bandgap (E_g) (eV)	Reference
1.	225	129	3.64	Present work
2.	300	300	3.91	Present work
3.	375	502	3.94	Present work
4.	150	400	2.87	Reference [8]
5.	300	400	2.47	Reference [8]
6.	350	400	2.07	Reference [8]
7.	400	400	2.05	Reference [8]

Photoluminescence and fluorescence Studies

Fig.6 shows the room temperature photoluminescence spectra of CdTe thin films coated at different substrate temperature recorded by Jasco Spectrometer FP – 8600. Intensity of the emission peak increases with increase in the substrate temperature for the films coated at 225 and 300˚C and the peak intensity decreases for the film coated at 375˚C. A strong photoluminescence peak is observed at 560 nm for the CdTe films coated at different substrate temperature. The position of the photoluminescence peak in the CdTe films coated from the synthesized CdTe slightly varies in the 532 – 578 nm range when the reflux time is increased from 1 to 18-h[24].

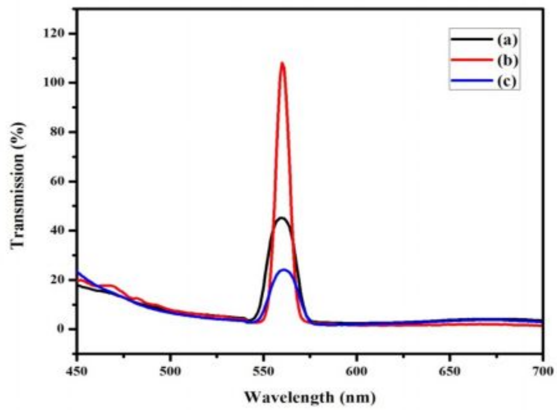


Fig. 6: Photoluminescence Spectra of CdTe film deposited at substrate temperature of (a) 225˚C, (b) 300˚C, (c) 375˚C.

Fig. 7 shows the fluorescence spectra of CdTe thin films coated at different substrate temperature recorded by Jasco FP- 6300 Spectroflurometer with 150 Watt Xe lamp.

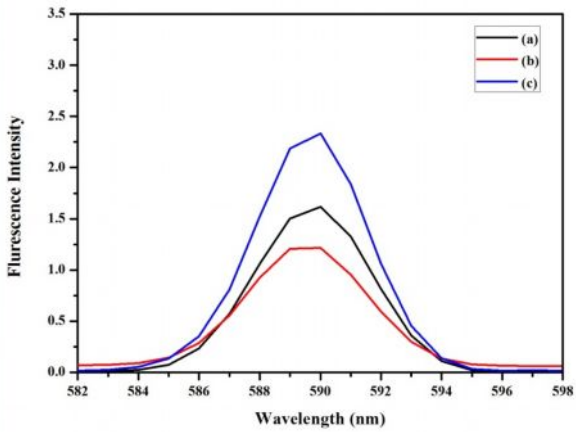


Fig. 7: Fluorescence spectra of CdTe film deposited at substrate temperature of (a) 225˚C, (b) 300˚C, (c) 375˚C.

Intensity of the emission peak decreases with increase in the substrate temperature from 225 to 300˚C and then increases for the film prepared at 375˚C. Fluorescence spectra of CdTe thin films show the emission peaks at 590 nm for the excitation radiation of 297 nm.

Conclusion

XRD peaks of the nanocrystalline CdTe thin films deposited by electron beam vacuum evaporation method at different substrate temperature 225, 300 and 375˚C confirm the cubic crystal structure. Intensity of XRD peaks increases with increase in the substrate temperature due to increase in the crystallite size. SEM images show the nanocrystalline nature of the deposited thin films. Elemental composition of the film shows that the films are rich in Te, due to relatively high vapour pressure of Te than that of the Cd. The transmittance of CdTe films decreases in the visible region for increase in the substrate temperature which may be increase in the film thickness with temperature. Optical band gap value of the coated films is relatively higher compared to that of the bulk material which may be due to Te rich in the films. Photoluminescence spectra of the films show a strong emission peak at 560 nm. Fluorescence of CdTe films is observed at 590 nm. Thus the present results reveal that the substrate temperature influences the structural, morphological and optical properties of the CdTe thin films.

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