Nanostructures, surface characterization and optical properties of chemically synthesized CdTe quantum dots

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Abstract: *Molar concentrations of chemical ingredients in synthesis of nanocrystals were found significant roles in the structural, surface morphology and visible range optical properties of CdTe quantum dots thin films. XRD, FESEM and UV spectrum analysis revealed that the average particle sizes approach 6-11nm quantum dots with increasing molar concentrations. The study of X-ray line profiles proved that peak intensity was increased with increasing of Cd^{+2} and Te^{2-} ions in the films. The phase structure of the films were found to possess cubic zinc blend structure with (100), (110), (200), (220) and (321) reflection planes at x = 0.1, 0.2, 0.4 and 0.6M and additional planes were also observed at x = 0.8M. In all the films, (200) reflection plane showed most prominent which facilitated estimation of nanoparticle sizes. The sized dependent nanoparticles showed maximum absorption blue shift near 325nm wavelength in ultraviolet regime ascribed as first excitonic transition. This may be attributed with decreasing particle sizes indicating increasing band gap.*

Keywords: *CdTe thin films, Quantum dots, XRD, FESEM, Optical properties*

I. Introduction

Polymerized nanocomposites (1-100nm) have versatile and diverse functions in terms of enhanced structural, optical, mechanical, magnetic and optoelectronic properties.[1, 2, 3] Cadmium tellurite belongs to II-VI compound semiconductors with bulk direct band gap of 1.5eV and has varied technological applications ranging from photovoltaic conversion, X-ray and v-ray detectors to electronic and optoelectronic devices because of its suitable to solar spectrum. Chemically synthesized semiconducting nanocrystalline thin films like CdTe are expected to show novel physical structures, optical and photoelectronic properties   different from their bulk counterparts as a result of three dimensional quantum confinement effect of excitons.[4] Basically, semiconductors with quantum dot nanocrystallites whose radii below bulk Bohr radius of 6nm constitute a class of material intermediate between bulk material and molecular form of material. [5,6] CdTe is also widely used as a buffer layer in infrared detectors using HgCdTe as the sensor element. Recent researchers reported that CdTe is considered for optical waveguide applications and has shown efficient photoluminescence properties at different frequencies depending on sized of the nanoparticles[7] .Several methods may be employed to fabricate CdTe thin layers such as thermal evaporation technique, closed space sublimation, electrodeposition, metal organic chemical vapour deposition,, chemical bath deposition (CBD).[8] Among these, CBD technique is chosen the best for deposition of CdTe thin films from echonomical and less time consumption to fabricate nanoparticles. The purpose of the present work is to study the effects of various chemical molar concentrations on the nanostructures, surface topology and optical properties of chemically deposited CdTe quantum dots at room temperature.

II. Experimental Detail

Synthesis of CdTe nanoparticles was carried out by means of chemical bath deposition technique at room temperature on ultrafine micro-glass slides at different molarities $0.1M \leq x \leq 0.8M$ using cadmium chloride ($CdCl_2$) as Cd-source and tellurium oxide (TeO) as the Te-source in double distilled water at p^H value 10. Equimolar solutions of $CdCl_2$ and TeO at 0.1M, 0.2M, 0.4M, 0.6M and 0.8M were prepared separately in double distilled water in highly cleaned glass beakers. The precursors were mixed in the ratio of 1:2 and stirred electro-magnetically for 30mins at room temperature. Ammonium hydroxide solution was added drop-wise until the solution became transparent. The p^H of the solution was measured and maintained at 10-11 by means of a high accuracy p^H-meter. 2 wt.% of PVA was prepared in highly cleaned glass beaker and stirred for 30mins at room temperature by means of magnetic stirrer till PVA matrix fully dissolved. Then 20ml of the PVA

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precursor was added to the above solution and stirred at 70^0C for 2 hrs using the magnetic stirrer until the solution became homogeneous, which was then thermally cooled down to room temperature. The chemically and ultrasonically cleaned glass substrates of proper sizes were immersed vertically in the matrix solution for 96hrs. The CdTe films deposited on the substrates were stabilized for 10mins and then washed with DD water several times for removal of unwanted film grains and then dried thermally at 10^0C above room temperature in oven for 24hrs.

III. Results and discussion
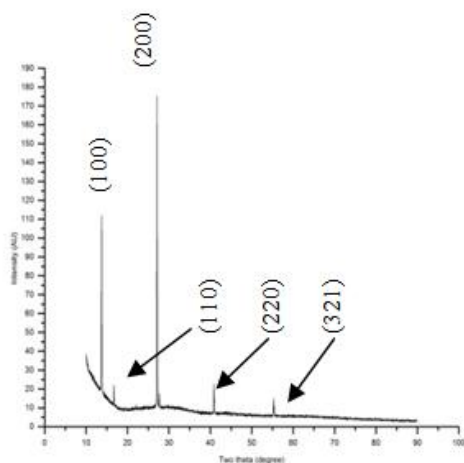
3.1.   Structural analysis

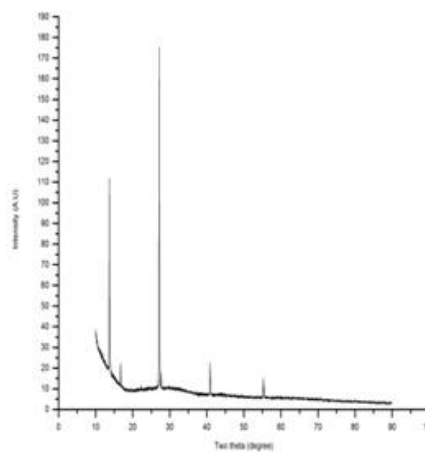Fig.1. XRD pattern of CdTe thin film at x = 0.1M

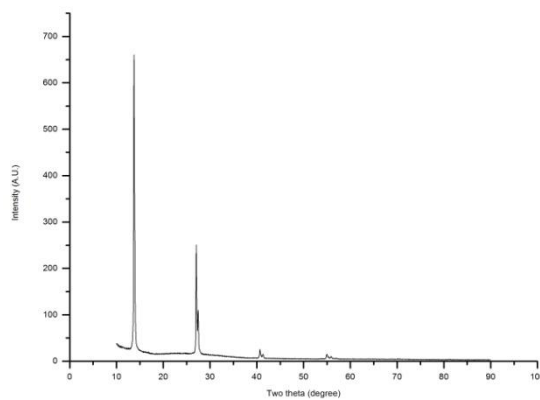Fig. 2. XRD pattern of CdTe film x = 0.2M

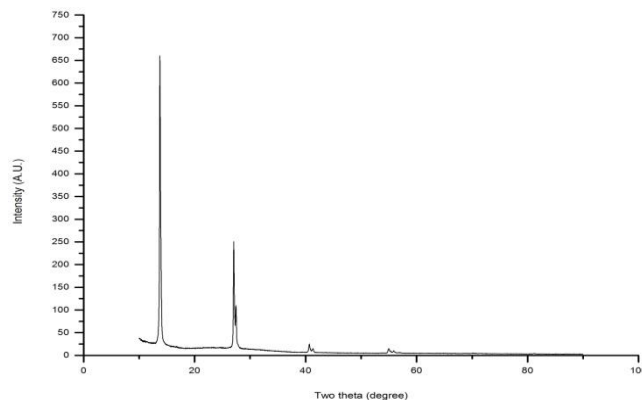Fig.3. XRD pattern of CdTe film at 0.4M.

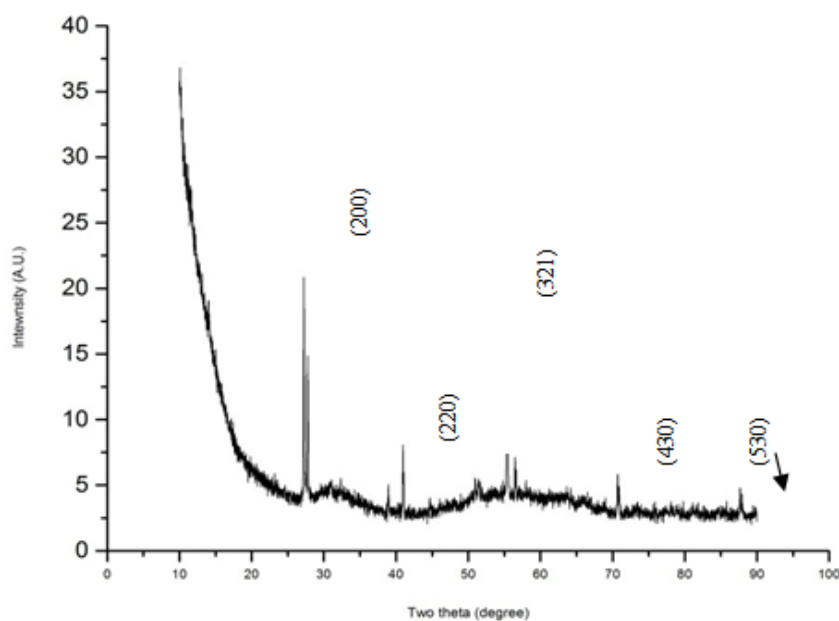Fig. 4. XRD pattern of CdTe film at 0.6M.
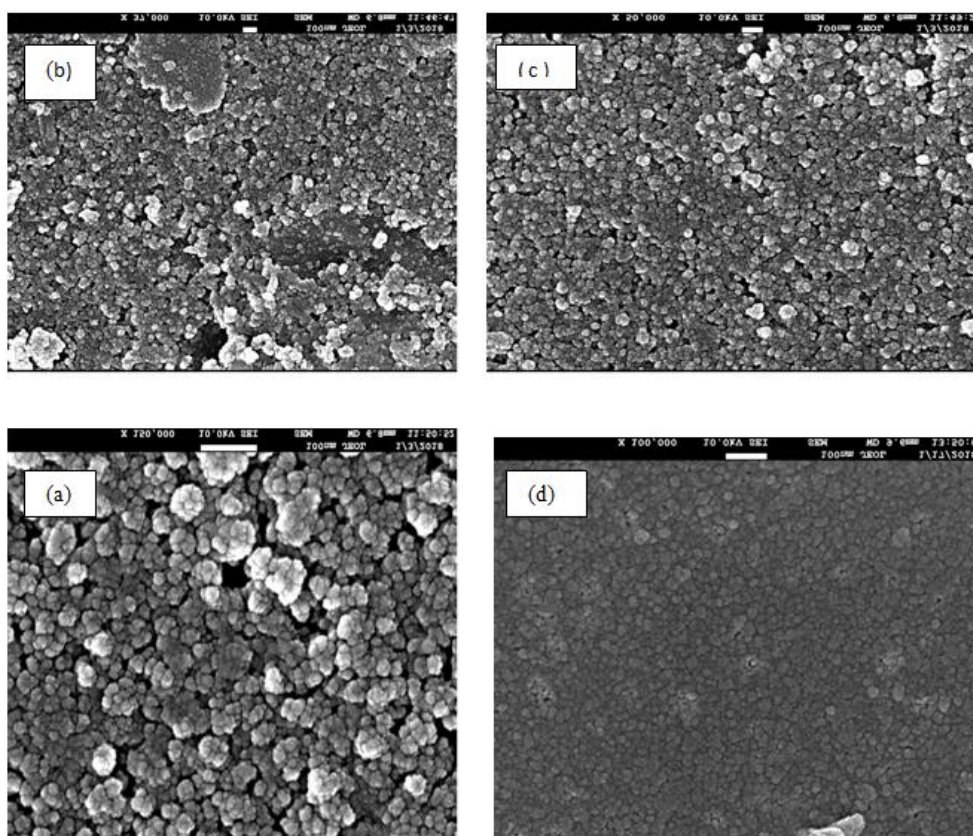
Fig. 5. XRD pattern of CdTe film at 0.8M.

Fig. 6. FESEM images of CdTe nanocrystalline films – (a) 0.2M (b) 0.8M (c) 0.4M (d) 0.6M.

Low angle X-ray diffraction patterns of the synthesized CdTe films at different molars were obtained by X-ray diffractometer (Phillips X'pert Pro-Automated Powder X-ray (model APD 1700) diffractometer with CuK$_{\alpha}$ – radiations (λ = 1.572Å)) and have been shown in Figures 1-5 while FESEM micrographs of the films in Figure 6. The diffraction patterns show the nanocrystalline growth of the films. Maximum peak intensity was

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found in 0.6M CdTe film grown at $2\theta = 14^{0.}$. The particle sizes in CdTe films grown at x = 0.1M, 0.2M,0.4M, 0.6M and 0.8M were calculated using D. Scherrer's relation [9]

$$D_{hkl} = k\lambda/\beta_{2\theta}Cos\theta \qquad\qquad -(1)$$

where the value of shape factor is 0.94, $\beta_{2\theta}$, the width of the peak at half of the maximum peak intensity and θ the Bragg angle. The estimated values of the particles sizes are shown in Table-1.

Table-1. Particle radius in synthesized CdTe films

Sl. No.	Molarity (M)	$2\theta_2$-value (degree)	$2\theta_1$-value (degree)	D_{hkl}-value (nm)
1.	0.1	28	27	6.11
2.	0.2	28	27	6.11
3.	0.4	14.5	13	11.44
4.	0.6	24	23	6.00
5.	0.8	29	27	6.01

The results show that the size of the particles in the synthesized CdTe films at different molars are in quantum dots regime. The lattice parameters of the phase structure of the grown CdTe films at different molar were calculated using the relation

$$d_{hkl} = a/\sqrt{(h^2 + k^2 + l^2)} \qquad\qquad -(2)$$

For first order reflection,

$$2dSin\theta = \lambda$$

for which

$$Sin^2\theta = \lambda^2/4d^2 = \lambda^2(h^2 + k^2 + l^2)/4a^2$$
$$=\lambda^2 N/4a^2 \qquad\qquad -(3)$$

where $N = h^2 + k^2 + l^2$, $\lambda = 1.54\text{Å}$ and $a = 6.48\text{Å}$ for bulk(**JCPDS-File 15-770**).

The (hkl) values and lattice parameters of CdTe nanocrystalline films at different molars and diffraction angles have been shown in Table-2. Five peaks at about diffraction angles 14,16,27,41 and 55 degrees were obtained corresponding to reflection planes (100), (110), (200), (220) and (321) with cubic phase structures at the growth molars 0.1-0.6M. The diffraction of X-rays were found most prominent in (200) plane at x = 0.1M, (200) plane at x = 0.2M, (100) plane at x = 0.4M and (100) plane again at x = 0.6M in CdTe films. With increase of source

Table-2. Lattice parameters and *hkl* –values of CdTe nanocrystals.

Molars (M)	I/I_0	2θ (degree)	hkl	JCPDS-*a*-value (Å)	a_{cal}-value (Å)	JCPDS *d*-value (Å)	d_{cal}-value (Å)
0.1	110	14	100	6.480	6.317	2.290	6.317
	21	16	110		7.824		5.533
	175	27	200		8.598		4.299
	20	41	220		6.226		2.202
	15	55	321		6.237		1.667
0.2	110.4	14	100	6.480	6.317	2.290	6.317
	20.1	16	110		7.824		5.533
	175.2	27	200		8.598		4.299
	20.3	41	220		6.226		2.202
	15.3	55	321		6.237		1.667
0.4	650	14	100	6.480	6.317	2.290	6.317
	......	....	.....		....		....
	248	27	200		8.598		4.299
	23	41	220		6.226		2.202
	16	55	321		6.237		1.667
	653	14	100		6.317		6.317
	......	....	.....		....		....

0.6	228	27	200	6.480	8.598		4.299
	24	41	220		6.226	2.290	2.202
	17	55	321		6.237		1.667
	......	.....	......		....		......
	......	......	......		....		......
0.8	22	27	200		8.598		5.533
	7	41	220	6.480	6.226	2.290	4.299
	18	55	321		6.237		1.607
	6	70.1	430		6.704		1.341
	5	88	530		6.460		1.108

molarity, CdTe nanocrystal showed prominent reflection from (200) plane at x = 0.8M corresponding to diffraction angle 27degree at lower peak intensity compared to others.

3.2. Study of optical properties in the films

The figure 7 shows the absorption *vs.* wavelength curves of the CdTe nanocrystals synthesized at different molars obtained from UV-vis. Spectrometer (model : Lamda 35LS 35, Parkin Elimer 2008 installed at NIT, Manipur). CdTe is a direct band gap semiconductor. The absorption coefficient, α in the films can be correlated to the photon energy as[10]

$$\alpha h\nu = A(h\nu - E_g)^{n/2} \qquad \text{- (4)}$$

where E_g is the energy band gap between the valence and the conduction bands, A is a constant being different for different transitions, and n is a constant being equal to 1 for direct band gap semiconductor.
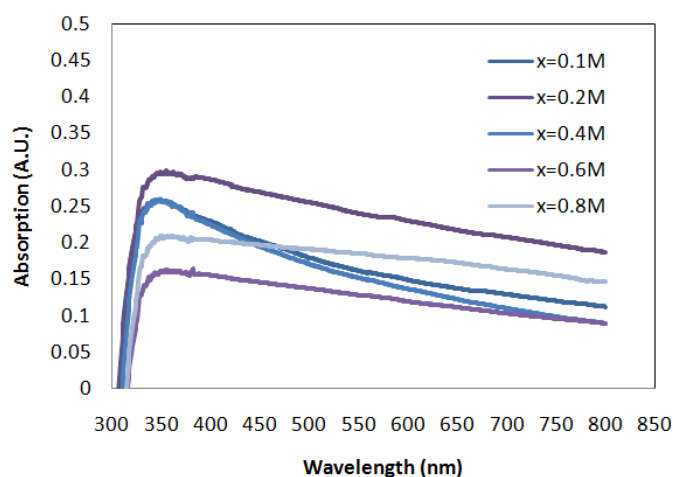
The absorption coefficient, α is found to enhance with increasing molar 0.2-0.6M within 312 – 800 nm wavelength range. The enhancement of the absorption in lower wavelength ranges may be attributed due to increase of agglomeration of quantum size nanoparticles under quantum size effect which absorb more photons of lower wavelengths with less transmissions. The study of the optical absorption spectra shows absorption peak at 350 nm which exits in the lower blue spectral side. The blue shift of the absorption edge indicates decreasing the grain sizes in the films [14]. The study of the optical band gaps with different molar concentration in the films shows an increase in band gap with increasing molars.
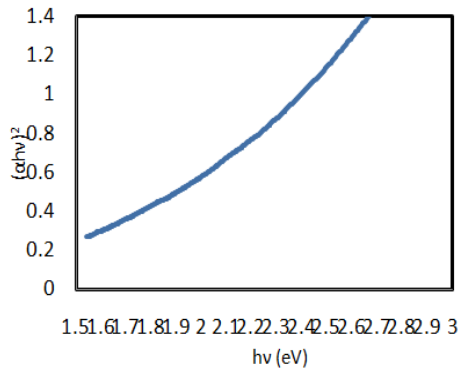
Fig. 8(a). *(αhv)² vs. hv* `curve of CdTe nanocrystal at 0.1M

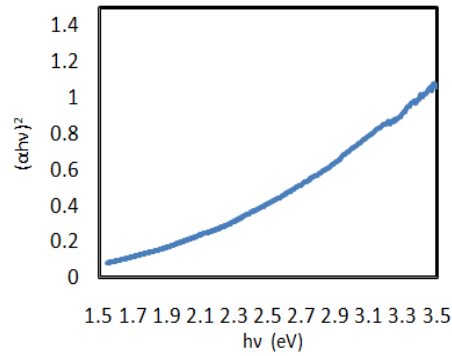Fig. 8(b). *(αhv)² vs. hv* curve of CdTe nanocrystals at 0.2M.
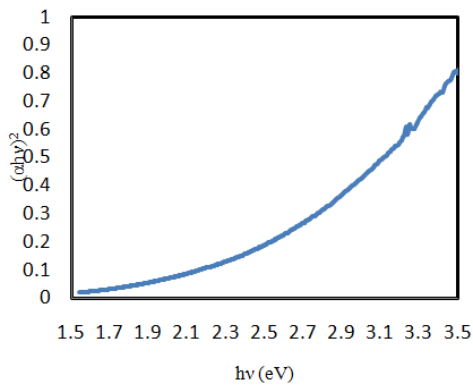
Fig.8 (c). *(αhv)² vs. hv* curve of CdTe 0.4M
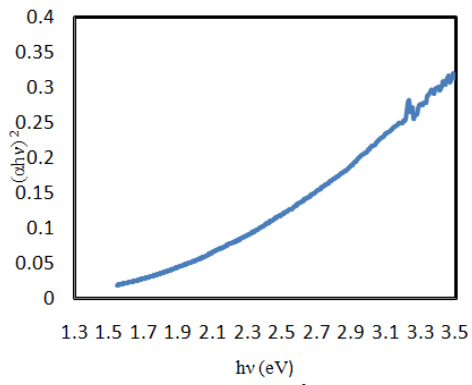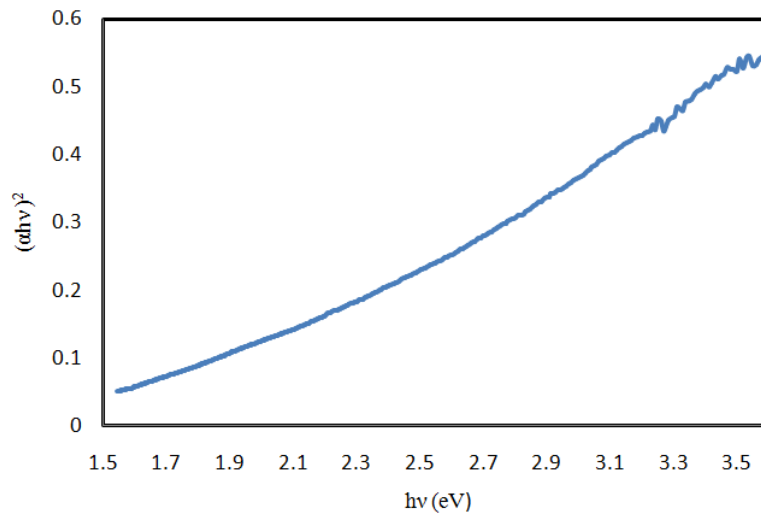

Fig. 8(d). *hv vs. (αhv)²* curve of CdTe nanocrystal at 0.6M.

Fig.8 (e). *hv vs. (αhv)²* curve of CdTe nanocrystals at 0.8M.

The increase in band gap in the films is a consequence of decreasing the crystallite sizes in the films. The change in the energy gap as function of crystallite or particle size in the films may be defined by a hyperbolic band mode[11] given by

$$E_{gn} = \sqrt{[\ E_{gb}^2 + 2h^2\ E_{gb}\ (\pi/R)^2/m^*]} \qquad\qquad - (5)$$

where E_{gn} is the band gap in nano-crystal films, E_{gb} the band gap in the bulk semiconductor, h the Plank constant, R the particle radius and m* is the effective electron mass. The eqn. (5) shows that energy gap increases with reduction in particle radius. The band gaps determined from $(αhv)^2$ *vs.* hv (photon energy) curves of CdTe filme at different molars with extrapolation to zero absorption as shown in Figures 8(a,b,c & d) have been shown in Table-3.

Table-3. Energy band gaps in CdTe films at different molars

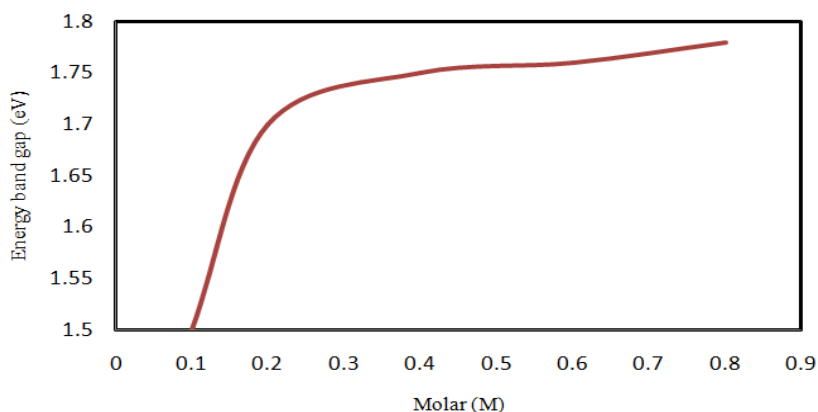| Molar (M)	E_g (eV)
0.1	1.5
0.2	1.7
0.4	1.75
0.6	1.76
0.8	1.78

Fig.9. Energy band gap vs. molar concentration curve of CdTe nanocrystals.

The variation of energy band gaps *vs*. molar concentrations of Cd^{2+} and Te^{2-} of CdTe films is shown in Fig. 9.The mechanisms of chemically deposited CdTe thin films at varied molars will find significant contributions in technological applications like fabrications of thin film solar cells, photo-detectors and many other photo-electronic devices.

IV. Conclusion

The chemically synthesized CdTe thin films at varied molars of Cd^{2+} and Te^{2-} ions at room temperature and deposition time are found enhancing in nanocrystalline growth with particle sizes within quantum dots. The phase structure of the films were found in cubic zinc blend structure with most preferential reflection along (200) plane at x = 0.1M, (200) plane at x = 0.2M, (100) plane at x = 0.4M and (100) plane again at x = 0.6M in CdTe films. With increase of source molarity, CdTe nanocrystal showed prominent reflection from (200) plane at x = 0.8M corresponding to diffraction angle 27degree at lower peak intensity compared to others. The optical analysis of the films reveals that the absorption coefficient, α is found to enhance with increasing molar. The enhancement of the absorption in lower wavelength ranges is expected due to increase of agglomeration of quantum size nano-particles under quantum size effect which absorb more photons of lower wavelengths with less transmissions. The absorption peak in the CdTe films were found at 350 nm which exits in the lower blue spectral side. The blue shift of the absorption edge indicates decreasing the grain sizes in the films. The study of the optical band gaps with different molar concentration in the films shows an increase in band gap with increasing molars.

Acknowledgement

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