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Characteristics $Cd_{0.3}Sn_{0.7}Se$ thin films as absorber materials for Solar cell devices

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Abstract

Cadmium Tin Selenide compound $Cd_{0.3}Sn_{0.7}Se$ was prepared by direct reaction of high-purity elemental Cadmium, Tin and selenium. $Cd_{0.3}Sn_{0.7}Se$ thin films were prepared on to well-cleaned glass substrates by vacuum thermal evaporation technique at room temperature of different thicknesses. The X-ray diffraction studies revealed that all the deposited films are amorphous in nature and exhibiting polycrystalline structure when are annealed at 348 K and 373 K. The crystallites were found to have a preferred orientation along the (111) direction. The analysis of its optical characteristics indicated the ability of these films to absorb the visible light due to its graded energy gap. As the thickness of the film and the annealing temperature increases, the optical band gap decreases. The absorption spectrum indicated that $Cd_{0.3}Sn_{0.7}Se$ films have maximum absorbance along the extreme of visible region especially for the thickness 690 nm. Therefore this property indicated that these films are considered as good absorber for solar cell devices.

Key Words: Methods, materials, CdSnSe

1. Introduction

Cadmium Tin selenide $Cd_{0.3}Sn_{0.7}Se$ is a promising material for thin film solar cells because of its ability to absorb the visible light due to its graded energy gap [1]. $Cd_{0.3}Sn_{0.7}Se$ is a semiconducting compound which belongs to ternary compounds of II, IV, and IV semi-conducting materials from the periodic table. $Cd_{0.3}Sn_{0.7}Se$ films possess certain exceptional material characteristics like band gap, absorption coefficient which are particularly suitable for photovoltaic applications [2].

A few workers studied CdSnSe compound by several techniques, such as Pathinettam et al. [3], who prepared CdSnSe compound in different ratios of its elements by co-evaporation of CdSe and SnTe powders and studied X-diffraction analysis. He recorded that those different ratios of compound crystallize in orthorhombic crystal system. Datta [4] prepared CdSnSe thin films by electrolysis deposition and he found that the structure of thin film is polycrystalline. Vacuum thermal evaporation has become a popular technique among different techniques available for the deposition of thin films. Vacuum thermal evaporation method yields high-quality thin films with smooth surfaces. Previously, our studies were made of $Cd_{0.3}Sn_{0.7}Se$ compound to investigate structural and electrical properties.We found that the compound has orthorhombic structure as detected by X-ray diffraction [5]. Its d.c. electrical conductivity is p-type and carrier concentration is 0.1×10^{12} cm^{-3} of gold electrodes for ohmic contact [6].

Aim of this research is to prepare $Cd_{0.3}Sn_{0.7}Se$ films by thermal evaporation at room temperature at different thicknesses and study the optical films were annealed at 348 K and 373 K temperatures.

2. Experimental

CdSnSe compound was synthesized in a quartz tube by taking cadmium metal, tin powder, and selenium powder in their respective stoichiometric ratios as 0.3, 0.7 and 1.0, respectively. The tube was evacuated then sealed. It was slowly heated in an electrical furnace at 1173 K and kept it at this temperature for 18 hours. The furnace was then left to cool at room temperature. Vacuum thermal evaporation was used to deposit $Cd_{0.3}Sn_{0.7}Se$ thin films at room temperature at 212, 451, and 690 nm thicknesses using an Edward E306A coating unit onto glass substrates, which were cleaned by distilled water, pure alcohol, and then by ultrasonic vessel in order to deposit thin films for structural and optical measurements. Thickness measurements were made by laser technique in Al-Mustansyria University. A molybdenum boat was used as the source holder and the pressure inside the chamber was better than 10^{-6} mbar The substrate was held at a distance of 12 cm exactly above the boat. The rate of deposition was 0.9 nm/s. Annealing of the thin films was conducted under vacuum, in oven at 348 K and 373 K, which are the available temperatures in our laboratory. X-ray diffractometer using Cu-Kα radiation, which operates at room temperature at a potential difference of 40 kV and a filament current of 20 mA, was used to measure XRD patterns for films.

A Shimadzu model UV-160 UV-Visible Spectrophotometer was used to measure the absorbance spectra in the range 200–900 nm for the thin films, before and after films were annealed at 348 K and 373 K temperatures.

3. Results and discussions

3.1. X-ray diffraction

Figure 1 shows the X-ray diffraction of the prepared $Cd_{0.3}Sn_{0.7}Se$ bulk. The sharp peaks present in X-ray diffraction indicate that the prepared $Cd_{0.3}Sn_{0.7}Se$ bulk is polycrystalline in nature. The preferred orientation of the particles are identified along crystallographic planes (210), (101), (201), (111), (020), (510), (121) and (610). Since there is no standard values available for $Cd_{0.3}Sn_{0.7}Se$ compound, XRD peaks were indexed as compared with the Pathinettam data. For more details, see reference [3].

X-ray diffraction of $Cd_{0.3}Sn_{0.7}Se$ thin films of different thicknesses deposited in the present study is shown in Figure 2. In the thin films the structure of $Cd_{0.3}Sn_{0.7}Se$ is amorphous in nature. The X-ray diffraction pattern of $Cd_{0.3}Sn_{0.7}Se$ thin films of 690 nm thickness annealed at 348 K temperature are found to exhibit polycrystalline structure as shown in Figure 3. But the other thicknesses (212 and 451 nm) remained in amorphous structure and this can be attributed to structural transformation with the growth of different sizes of grains because of thicker films have more atoms in the film. Miller indices of different peaks in Figure 3 are indicated in Table 1 as well as values of inter-planar spacing d. These data are in good agreement with data in reference [3].

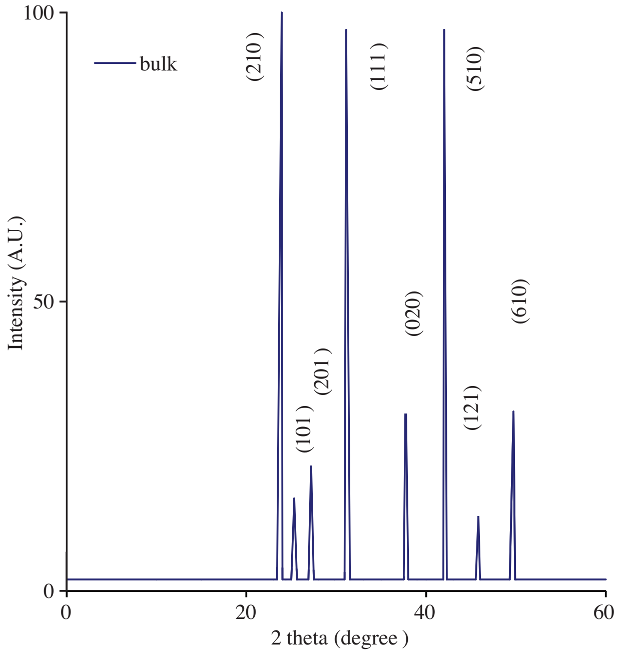

Figure 1. XRD patterns for $Cd_{0.3}Sn_{0.7}Se$ bulk crystal.

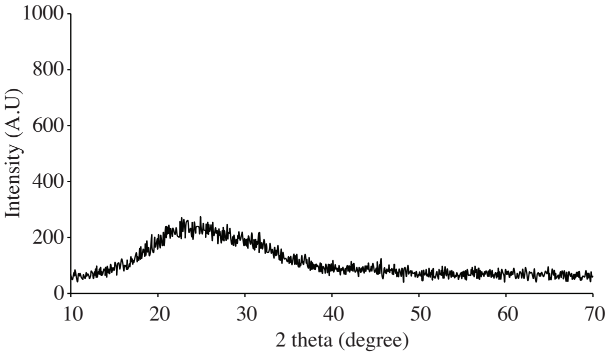

Figure 2. XRD for $Cd_{0.3}Sn_{0.7}Se$ thin films deposited at room temperature for all thicknesses.

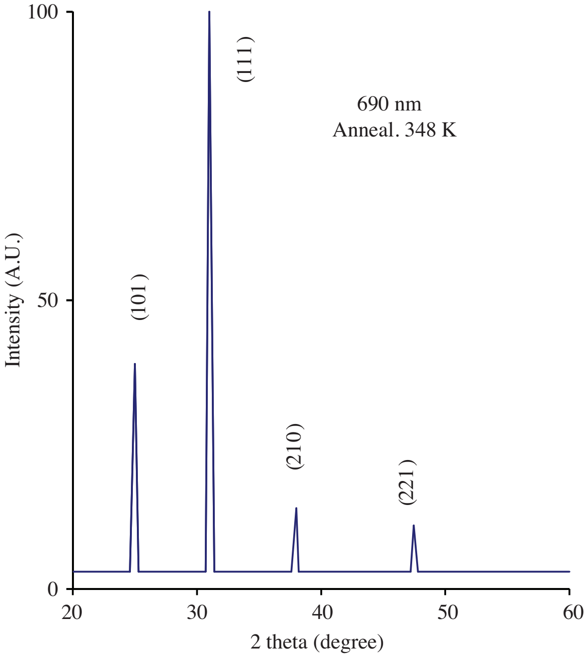

Figure 3. X-ray diffraction data for annealed $Cd_{0.3}Sn_{0.7}Se$ thin films at 348 K for 690 nm film thickness.

Table 1. X-ray diffraction data for annealed $Cd_{0.3}Sn_{0.7}Se$ thin films at 348 K for 690 nm film thickness.

(hkl) Plane	2θ (degrees)	d_{exp}(Å)	$(I/I_o)_{exp.}$
(101)	25.00	3.630	39
(111)	30.999	2.890	100
(020)	37.999	2.373	14
(221)	47.471	1.910	11

As the annealing temperature increased to 373 K, the 451 nm films were found to show polycrystalline structure, as indicted by the X-ray diffraction pattern shown in Figure 4. A additional diffraction peaks appeared for films of 690 nm thickness after films were annealed at 373 K, as shown in Figure 5. But the other thickness of 212 nm is stayed in amorphous structure. This is due to the increase of grain size and can be explained to the movement of atoms after annealing to array its selves in different sizes of grains. Miller indices and inter-planar spacing for peaks in Figures 4 and 5 are indicated in Table 2.

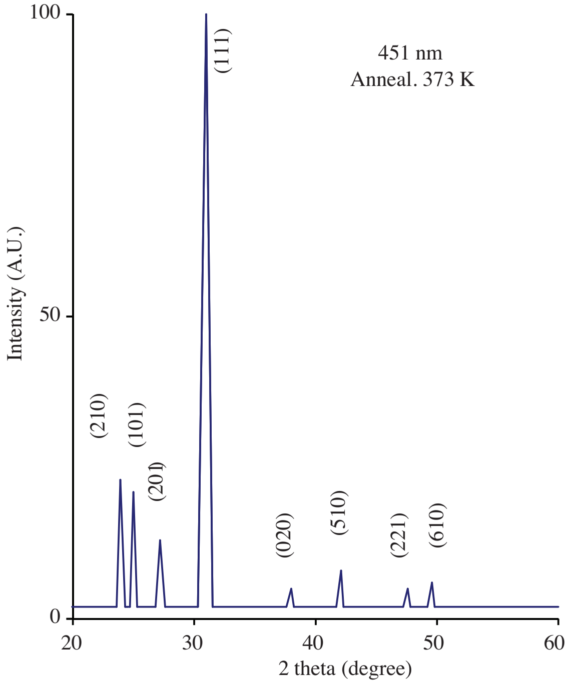

Figure 4. X-ray diffraction data for annealed $Cd_{0.3}Sn_{0.7}Se$ thin films at 373 K for 451 nm film thickness.

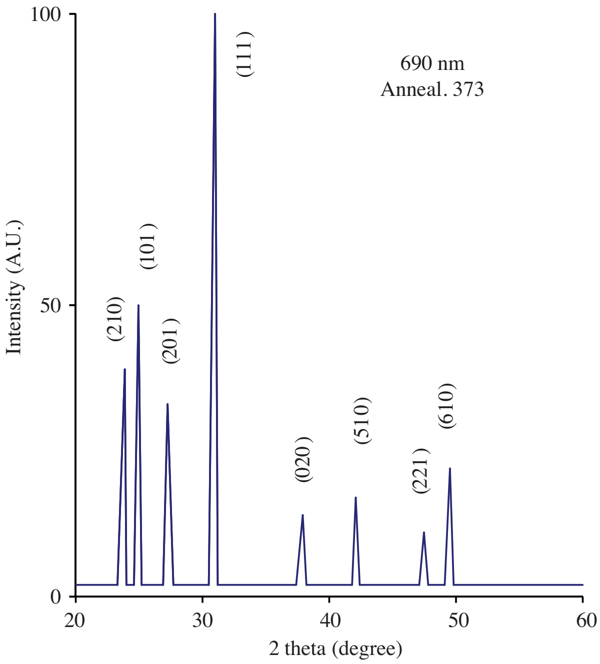

Figure 5. X-ray diffraction data for annealed $Cd_{0.3}Sn_{0.7}Se$ thin films at 373 K for 690 nm film thickness.

3.2. Optical properties

3.2.1. Absorbance spectra

The absorbance spectra of $Cd_{0.3}Sn_{0.7}Se$ thin films of different thickness deposited at room temperature is shown in Figure 6. All the deposited $Cd_{0.3}Sn_{0.7}Se$ thin films show maximum absorbance at the beginning of 325 nm wavelength. The overall absorbance increases with increase of film thickness for the same reason that of thicker films: that more atoms present in the film means more states will be available to absorb the photons.

Absorbance spectra for annealing films at 348 K and 373 K shows different behavior that the maximum of the absorbance shifts towards the longer wavelengths as shown in Figures 7 and 8, and this suggests the decrease in the band gap with the increase of film thickness and grains size [7, 8].

Table 2. XRD data for annealing $Cd_{0.3}Sn_{0.7}Se$ thin films at 373 K for film thicknesses 451 nm and 690 nm.

Thickness, (nm)	(hkl) plane	2θ (degree)	d_{exp} (Å)	$(I/I_{\bigcirc})$, experimental
451	(210)	23.918	3.714	23
	(101)	24.990	3.645	21
	(201)	27.190	3.234	13
	(111)	30.990	2.910	100
	(020)	37.990	2.357	5
	(510)	42.092	2.145	8
	(221)	47.590	1.900	5
	(610)	49.580	1.850	6
690	(210)	23.874	3.733	39
	(101)	24.960	3.654	50
	(201)	27.250	3.244	33
	(111)	30.989	2.900	100
	(020)	37.910	2.364	14
	(510)	42.090	2.149	17
	(221)	47.470	1.912	11
	(610)	49.510	1.854	22

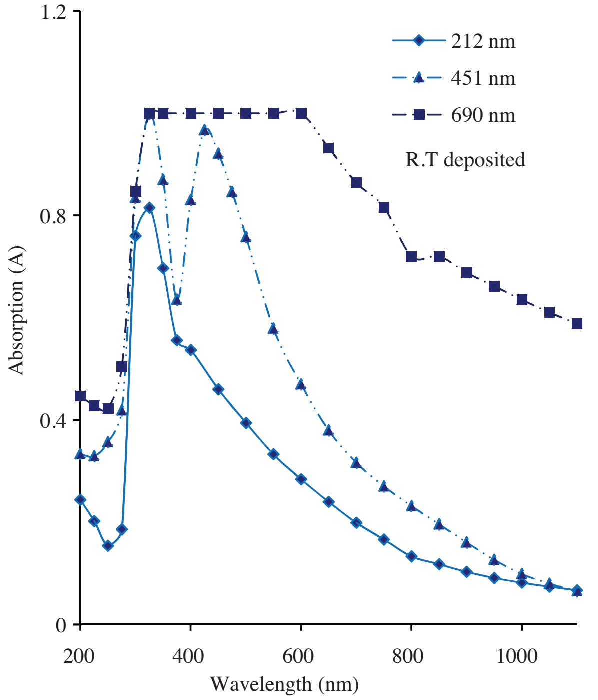

Figure 6. Absorbance spectra for $Cd_{0.3}Sn_{0.7}Se$ thin films deposited at room temperature.

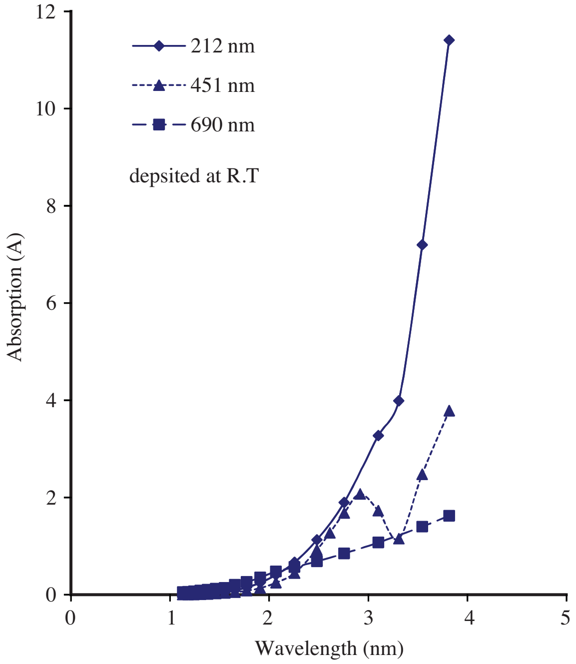

Figure 7. Absorbance spectra for $Cd_{0.3}Sn_{0.7}Se$ thin films after annealing at 348 K.

3.2.2. Optical energy gap

The absorption coefficient has been determined and is found to be of the order of 10^4 cm^{-1}. The electronic transition between the valance and conduction bands can be direct or indirect. In these two cases, the transition of electron can be allowed as permitted by the transition probability n or forbidden where no such probability exists. The transition probability is given by [8]

$$(\alpha hv)^n = A(hv - E_g), \tag{1}$$

where E_g denotes the band gap, $h\nu$ is the energy of the incident photon and A is a constant independent of the transition type. The exponent n is a number which characterizes the transition process. The nature of transition in the film can be determined by plotting $(\alpha hv)^n$ against photon energy hv for suitable value of n which yields straight line behavior. The band gap E_g is determined by plotting $(\alpha hv)^n$ against photon energy hv for suitable value of n where the graph is a straight line and the value of E_g is obtained by extrapolating the linear portion of the graph to intercept the photon energy axis. Since there is no straight line behavior in the plots for $(\alpha hv)^{2/3}$ versus hv (direct forbidden), $(\alpha hv)^{1/2}$ versus hv (indirect allowed), $(\alpha hv)^{1/3}$ versus hv (indirect forbidden), the type of transition is neither direct forbidden nor indirect. The presence of a single slope in the curves in the plot of $(\alpha hv)^2$ versus hv of $\mathrm{Cd}_{0.3}\mathrm{Sn}_{0,7}\mathrm{Se}$ thin films suggests that all the films are single phase in nature with direct-allowed transition. The energy gap of the films has been determined by extrapolating the linear segment of the plots drawn for $(\alpha hv)^2$ versus hv to the energy axis, as shown in Figures 9, 10 and 11 for all film thicknesses as deposited and at annealing temperature. Two values of optical energy gap are shown in Figure 9 for 451 nm film thickness deposited at room temperature; and this is due to the polycrystalline structure which has different grains size [9, 10]. Table 3 gives the optical band gap of $\mathrm{Cd}_{0.3}\mathrm{Sn}_{0.7}\mathrm{Se}$ thin films of different thicknesses deposited at room temperature and annealing temperature 348 K and 373 K. It clearly shows that as thickness of the film increases the optical band gap decreases. The decrease in energy band gap with the thickness may be attributed to an increase in particle size and decrease in strain.

Table 3. Values of energy gap as a function of film thickness at room temperature and annealing temperatures.

Thickness (nm)	Energy Gap (eV)		
	Room	Annealing Temperature	
		348 K	373 K
212	3.0	2.2	1.8
451	2.1 – 3.0	2.4	1.7
690	1.5	1.7	1.6

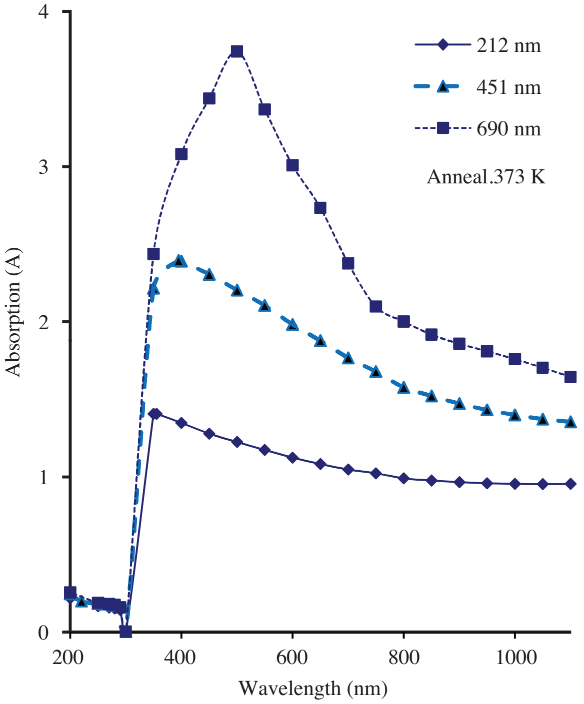

Figure 8. Absorbance spectra for $Cd_{0.3}Sn_{0.7}Se$ thin films after annealing at 373 K.

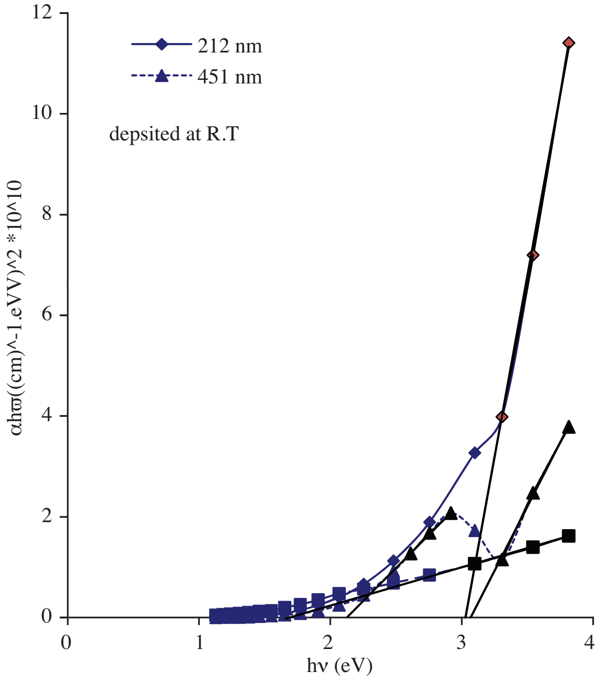

Figure 9. Absorption coefficient for $Cd_{0.3}Sn_{0.7}Se$ thin films deposited at room temperature.

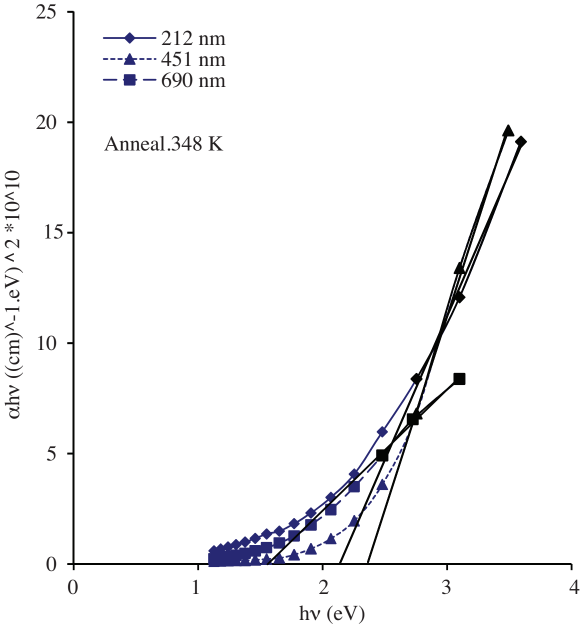

Figure 10. Absorption coefficient for $Cd_{0.3}Sn_{0.7}Se$ thin films annealing at 348 K.

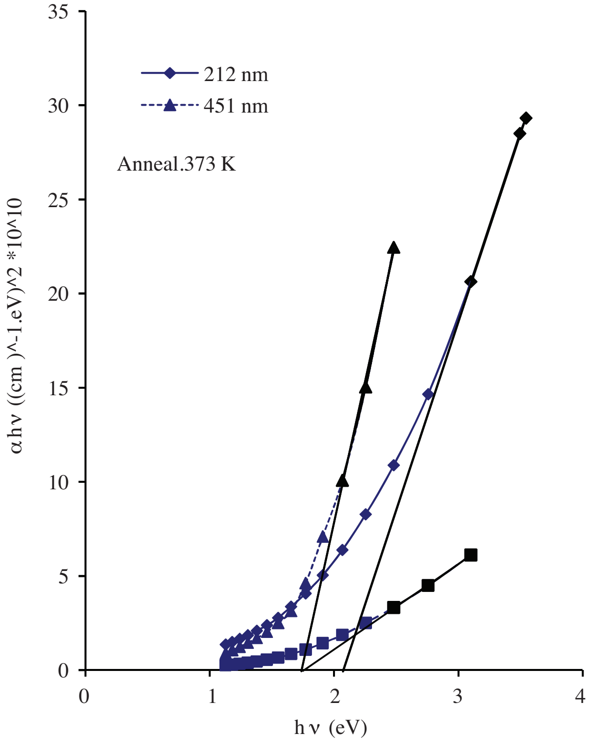

Figure 11. Absorption coefficient for $Cd_{0.3}Sn_{0.7}Se$ thin films annealing at 373 K.

4. Conclusion

CdSnSe thin films were prepared by thermal evaporation method at room temperature at thicknesses 212, 451 and 690 nm. Thin films for all thicknesses have amorphous structure, as investigated by XRD. Films have polycrystalline structure after films were annealed at 348 K and 373 K. From the results all the films, which were deposited at room temperature, have maximum absorbance at the beginning of 325 nm wavelength. The overall absorbance increases with the increase of film thickness. After films were annealed at temperatures 348 K and 373 K, the maximum of the absorbance shifts towards the longer wavelengths and this suggests the decrease in the band gap with the increase of film thickness and grains size. Two values of optical energy gap for 451 nm film thickness deposited at room temperature. From optical measurements, the deposited films at room temperature are considered as good absorber for visible light for devices like solar cells. Also after films were annealed at temperatures 348 K and 373 K, thin films are good absorber for infrared radiation for devices like sensors.

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