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Studies on the Structural and Conduction mechanism (ac) in thermally Evaporated CdSe thin films

K S Rajni

Amrita School of Engineering, Amrita Nagar, Coimbatore-641112, India

Abstract : In the present work, the structural properties of thermally evaporated CdSe films prepared at different thicknesses has been undertaken and the conduction mechanism is studied for the film of thickness 100nm. It is noted from the result that, all the films prepared at room temperature are poly crystalline and the peak oriented towards (002) plane and the peak corresponding to (103) plane begins to emerge when the thickness increases. From the analysis of the ac conductance mechanism, it is noted that it varies according to the relation Gp α ω^n and'n' is found to vary depending on the frequency and temperature range studied, which suggests that the conduction mechanism in CdSe thin films are by means of hopping.
Keywords: Structural and Conduction mechanism (ac), thermally Evaporated, CdSe thin films.

Introduction

Among the II-VI compound semiconductors CdSe is a promising candidate because of its potential application in photoconductive and photovoltaic cells, thin film transistors, lasers, optoelectronic devices. CdSe nanocrystalline films can be used as photo electrodes in photo electrochemical cells with relatively low recombination losses. CdSe is a direct bandgap semiconductor (1.72eV) which has high photosensitivity and has a suitable bandgap that matches with the maximum solar spectrum. Also it observed that for the efficient utilization of these materials for the devices, the electrical and optical properties of these materials are tuned by changing the thicknesses, preparing the films at different substrate temperatures and also changing the preparation conditions. In the present work CdSe thin films are prepared at different thicknesses (100, 200,300 and 500nm) by vacuum evaporation technique at a pressure of 10^{-5} Torr onto the glass substrate at room temperature. The microstructural and the ac conduction mechanism were analyzed for the prepared films and the results were discussed.

Experimental

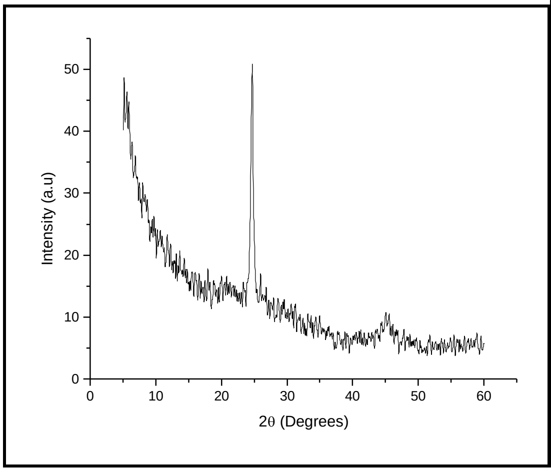
CdSe thin films are prepared by thermal evaporation of CdSe polycrystalline powder under a pressure of 10^{-5} Torr vacuum. Well cleaned glass slides are used as the substrate and they are kept at a distance of approximately 20.0 cm from the source. The flow rate is maintained at 4.5 A^0 /s and molybdenum boat is used. Thin films are prepared at different thickness ranging from 100 nm to 500 nm and are verified by multiple beam interferometer (forming fizeau's fringes) technique. The micro structural properties of the as deposited thin films were analyzed by the X-ray diffractrometer (JEOL 8030, using Cu Kα radiation with λ =0.1541 nm). The optical transmittance of films are recorded using UV-Vis-NIR spectrophotometer (Jasco Corp., V-570) in the wavelength region of 300-1110nm.Using the digital LCR meter (LCR-819,GW instek, Goodwill instrument company Ltd., Taiwan) series capacitance and dissipation factor in the frequency range of 100Hz to 100KHz were carried out at various substrate temperatures (303-483K) in a rotary vacuum system (10^{-3} mbar). The dielectric constant was evaluated from the known area and thickness of the dielectric films. The parallel equivalent conductance Gp (= ω C_p tanδ) was calculated at different temperatures from the measured values of C and tan δ.

Results and Discussions

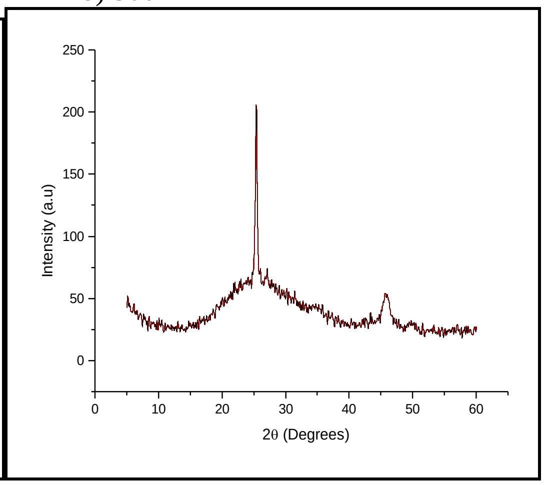
Structural analysis

The XRD analysis proves that all the as deposited CdSe thin films exhibit polycrystalline nature with Wurzite structure. The fig 1(a-d) shows that, in all the thicknesses the diffraction peak for (002) plane is prominent and the peak corresponding to (103) begins to emerge. The other low intensity peaks shows the development of coarsely fine crystallites (or) nanocrystallites in the prepared thin films. This shows that the at initial stages of thin film formation , the atom are deposited at random fashion and as the thickness increases the poly crystalline grain begins to orient more along (002). Similar nature was found in hot wall deposited CdSe films By Velumani et al[1]. In the present investigation tuning to (103) direction is also seen.

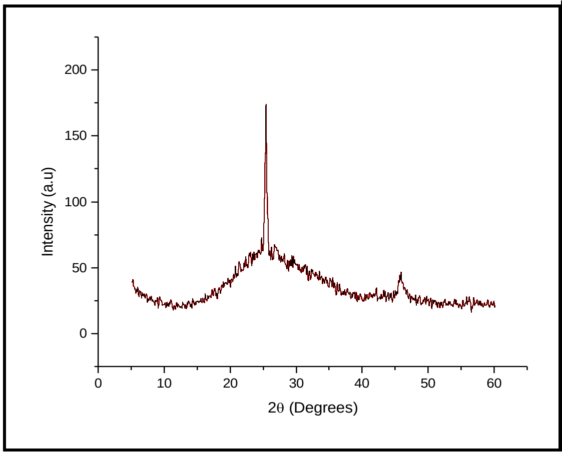
a) 500nm



b) 300nm



(c)200nm



d)100nm

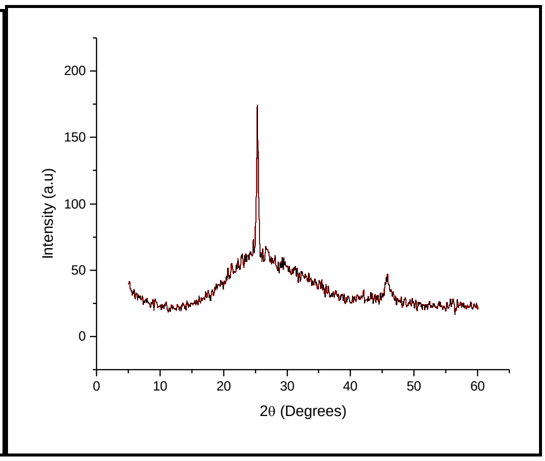


Fig 1-X-ray diffractrogram of CdSe thin films prepared at thicknesses of(a)500nm,(b)300nm,(c)200nm and (d)100nm

Table-1 Microstructural parameters of as deposited film with different thicknesses

t(nm)	d(nm)	D(nm)	ρ (x^{15})lines/m^2	ε 10^{-4}	N ($x10^{15}/m^2$)
100	3.5033	21.5	2.16	3.74	6.04
200	3.5259	28.1	1.27	2.81	9.01
300	3.5287	29.1	1.18	2.7	12.2
500	3.595	23.1	1.87	3.42	40.5

The table (1) shows the comparative values for the various microstructureal parameters of CdSe thin films coated on the glass substrate for various thicknesses. It is noted that the dislocation density (ρ) and the strain (ε) decreases with increase of film thickness up to 300 nm and after that an increase in the dislocation density and strain were observed. A similar trend was observed by Pal et al[2] for vacuum deposited CdSe films and Velumani et al[1] for hot wall deposited films. In the present investigation for 500nm thickness the bandgap is 1.72eV with the grain size of 23.1 nm is obtained. The increase in grain size with particular thickness and decrease thereafter is attributed to the formation of new smaller grains on the larger films. The size of the grain does not increase indefinitely with thickness but reaches a level where average grain size begins to oscillate with increase of thickness and it becomes difficult to analyses experimentally as observed for PbTe films[3]

The variation in optical bandgap with thickness is as shown in the fig (2).

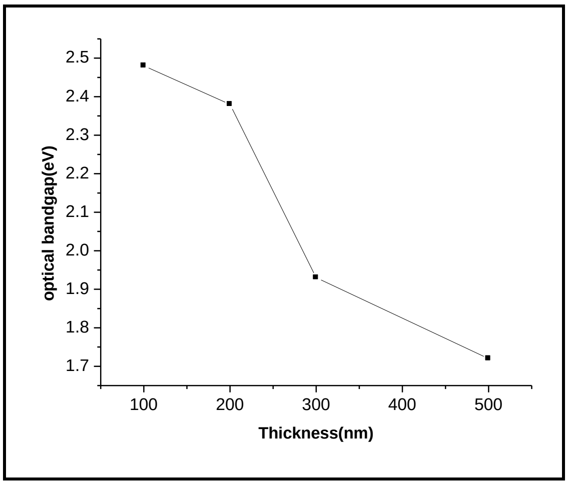


Fig 2 Optical bandgap Vs Thickness

In semiconductor and semi metal films the quantum size effect appears when the thickness of the film is comparable with the mean free path and the effective De Broglie wavelength of the carriers. The transverse component of the quasi-momentum of the carrier is quantized due to the finite size of the thickness. Therefore the transverse component of the electron states assumes quasi-discrete energy values in this film. Due to this quantization the bottom of the conduction band and top of the valence band are separated by an additional amount of energy which is given by Δ E[4].

$$\Delta E = h^2/8m * t^2$$

The variation of energy gap for as deposited film with $1/t^2$ is shown in the fig. (3) It is found that the graph is linear and the decrease in the band gap energy and also the additional amount of energy with increase in the thickness of the film is attributed to the quantization effect[5]. The intercept with the Y axis is I.72eV which is the energy gap value for the bulk. In this study the optical bandgap decreases with the increase in thickness is due to quantum size effect which is verified by the linearity of the in the fig(3).the optical bandgap shows straight line up to 300nm which is comparable to mean free path and the effective de-Broglie wavelength of the carrier[6].

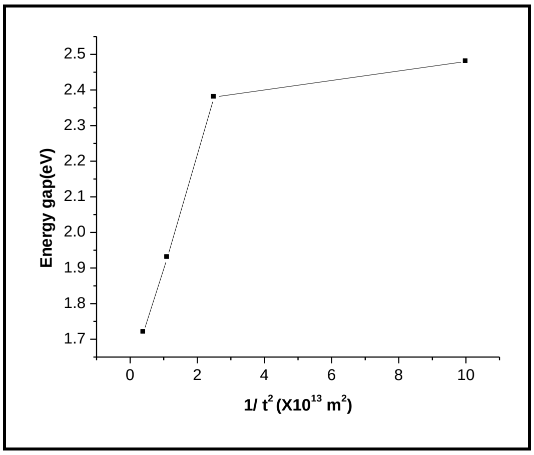


Fig 3. Variation of Eg with 1/t2

Table.2 Variation of Δ E with thicknesses

S.No	t(nm)	Eg (eV)	∇E (eV)
1	100	2.48	1.15
2	200	2.38	0.286
3	300	1.93	0.127
4	500	1.72	0.0458

This type of three dimensional quantum size effects where the band gap increases with the decrease in the particle size is well known for colloidal semiconductor sols where the individual colloidal particles are dispersed in a liquid or glass[7].

AC conduction studies:

As the properties such as structural, optical and conduction behavior of thin films varies with their bulk counterpart, first thin films are prepared and their average grain size are analyzed and the conditions are optimized for the investigation on the conduction nature of thin film. In the present work as the nature of conduction is same for almost all the thicknesses, thin film of thickness 100nm is taken for study. In general, three types of conduction mechanisms provide the current conduction through polycrystalline thin films such as thermionic emission, tunneling and hopping mechanisms which dominate the current conduction at highest to lowest temperature regions. Similar to the single crystal semiconductors, polycrystalline semiconductors have valance and conduction bands. Space-charge regions between grains bend these bands and create potential barriers to current carriers. The *ac* bias voltage never exceeds a few hundred millivolts which lead to the appearance of more than one conduction mechanism being active. This helps to understand the difference between localized and free band conduction. This helps to understand the difference between localized and free band conduction. In the case of localized conduction the conductivity ($\sigma_{a.c}$) increases with frequency ω, while in the free band conduction the conductivity decreases with frequency. It has been pointed out by Elliott[8] that variety of conduction mechanisms can yield the ωs behaviour for the a.c. conductivity, but in general, it is difficult to establish which of the above effects determines a given observed conduction process. A careful study of the temperature dependence of *s* (*s* is an index) can provide us more information in order to make a choice between the different theories for explaining the law $\sigma_{a.c(}\omega) \propto \omega_.$ The ac conductance can be calculated using the relation

$$\sigma = \omega C \tan\delta$$

where C is the measured capacitance, ω is the frequency and $\tan\delta$ is the loss factor. Fig (1) shows the I-V characteristics of CdSe thin film prepared at room temperature at a thickness of 100nm. It is noted that the prevalent conduction mechanism is non ohmic in nature. To identify the conduction mechanism, the graph has to be analysed since the nonlinearity is exhibited by different conduction mechanism. The nonlinearity can be explained in terms of either Richardson-Schottky[9] or Poole-Frenkel[10]. In the Schottky emission type, the conduction is by field assisted thermal excitation of electrons are observed. The electrons are transported from the cathode into the conduction band of the contact barrier. In the case of Pool-Frenkel emission, electrons may be transported by field-assisted thermal excitation over the lower coulombic potential barrier.

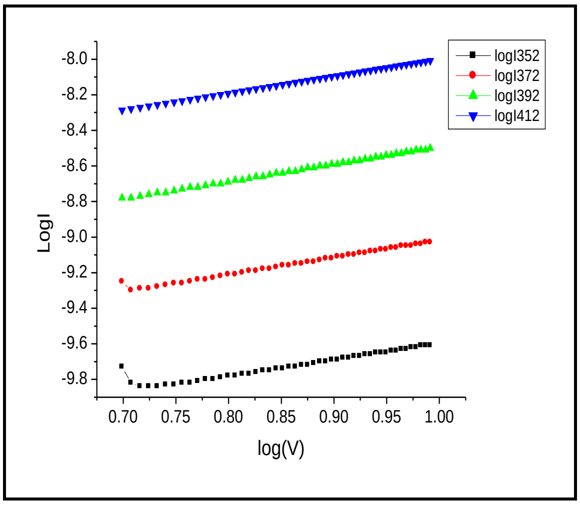


Fig3. Variation of current as a function of voltage at different temperatures in a CdSe thin film of thickness 100nm

Fig (4) shows the plot of ac conductance verses frequency. It is noted that the ac conductance has been found to vary according to the relation Gp α ω^n and 'n' is found to vary depending on the frequency and temperature range studied. The curve exhibits two dispersion region one below 900Hz and the other above 900Hz. In the second region all the curves approximate to a square law dependence on frequency and show less dependence on the temperature at higher frequencies. This suggests that the conduction mechanism in CdSe thin films are by means hopping and similar behavior is observed by various investigators[11,12] on insulating dielectric thin films. In the first region the slope of the curve is found to be less than 2 and it is found to be temperature sensitive. The value of n is found to decrease with increase in temperature. This is due to the fact that as the carrier movement between and within the defect levels are different at different a temperature which leads to the variation in carrier movement for contribution the conductivity. This behavior suggests that the mechanism responsible for conduction is of hopping type and it is consistent with the result reported by various hopping systems. It is noted from the fig that a.c conductivity increases with the frequency which is attributed to the localized conduction[12]. Also this trend increases with temperature. This type of behavior is observed in various other metals[13-15].

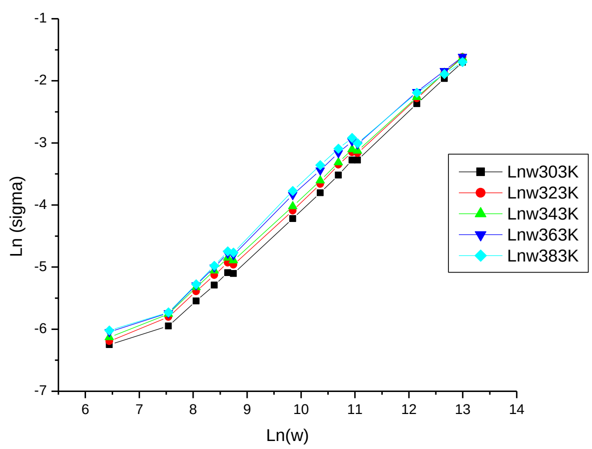


Fig 4. Variation of *ac* conductivity with frequency at different temperatures in a CdSe thin film of thickness 100nm

The conductivity is calculated for the temperature range of 303-403K in the frequency range of 1Khz to 70kHz and the graph is plotted for Ln(σ) Vs 1000/T for the frequency 1kHz and it is noted that the conductivity is the linear function of reciprocal of temperature (Fig 5). It is noted that the conductivity increases with the temperature and the plot is same for all the frequencies. The activation energy is calculated from the slope of the curve using the formula and it is found to 0.0951eV.

$\sigma = \sigma_0$ e $(-Ea/k_BT)$.

Where σ σ_0 is the pre exponential factor depending the nature of the material, Ea is the activation energy, k_B is the Boltzmann constant and T is the absolute temperature

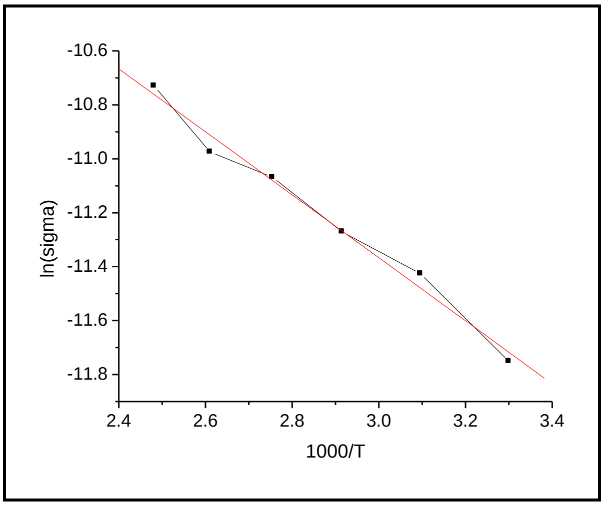


Fig 5 Variation of ac conductivity with temperature in a CdSe thin film of thickness 100nm

Conclusion

Cadmium selenide thin films prepared by thermal evaporation technique shows crystalline nature with (002) orientation. It is noted from the conduction studies that at low frequencies and at higher temperatures, the capacitance is dependent on both temperature and frequency and it is independent on frequency at low temperatures and higher frequencies. Analysis shows that the conduction mechanism is by means of hopping.

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