

Structural properties for cadmium selenide thin films deposited by thermal evaporation technique

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CdSe, belongs to group II-VI semiconductors, is found to be promising material for its applications in the area of electronics and opto-electronics. The structural properties of CdSe thin films have been investigated. CdSe thin films have been deposited on suitably cleaned glass substrates by thermal evaporation method for different thickness 150 nm, 200 nm, 250 nm and 300 nm. Polycrystalline nature of the material was confirmed by X-ray diffraction technique and various structural parameters were calculated. All the films show most preferred orientation along (0 0 2) plane. The grain size of deposited CdSe films is small and is within the range of 26 to 40 nm.

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1. Introduction

Binary semiconductor compounds belonging to II–VI groups of the periodic table are important due to their potential used in photoconductive devices and solar cells [1–4]. Among the II–VI group elements, CdSe is an important material for the development of various modern technologies of low cost devices such as light emitting diodes, solar cells, photodetectors, electrophotography, lasers and high-efficiency thin film transistors etc. [1]. CdSe is one of the prominent materials due to its near optimum direct energy gap in the range of 1.65 eV–1.84 eV has been reported by various authors [5] and high absorption coefficient. High quality CdSe thin film can be fabricated by several techniques such as electro deposition, evaporation [6–7] and chemical bath deposition [8–9]. Optical and electrical properties of semiconducting films are essential requirements for proper applications in various optoelectronic devices. These properties of the films are generally structure sensitive. The structural parameters such as lattice constant, grain size, etc. are dependent on the deposition conditions. The structure of CdSe thin films is dependent on the rate of deposition, substrate temperature, vacuum conditions, film thickness, etc [6]. In the present investigation, thermal evaporation method of cadmium selenide thin films has been reported. Structural characterization from XRD was carried out.

2. Experimental procedure

Thin films of CdSe having thickness around (150–300) nm were deposited by using vacuum coating unit type (Edwards Speedvac Unit). Test glass slides, cleaned by alcohol with ultrasonic waves in order to remove the impurities and residuals from their surfaces.

The cleaning of glass substrates is very important process because the influences like oil or dust affect on the thin films properties. First of all, the gadgets of the

vacuum chamber were cleaned by acetone. A clean evaporation source – molybdenum boat – was fixed in the filament holder inside the chamber. Stoichiometric CdSe powder having purity around 99.99 % was kept in a molybdenum boat. The substrates were cleaned first by acetone. The chamber was evacuated at a pressure better than 10^{-5} Torr by the combination of rotary and diffusion pump. When 10^{-6} Torr vacuum was attained in vacuum chamber, the heater was connected to the evaporation source was switched on which in turn slowly heated the source of CdSe to temperatures greater than the melting point. This allowed the evaporation of CdSe material. The thickness of the deposited films was obtained from light-beam Fizeau fringe method.

The structural properties were determined by X-ray diffraction (XRD) using $\text{CuK}\alpha$ radiation of wave length 1.54056 \AA at 300 K.

3. Results and discussion

Structural properties

The structural elucidations of CdSe film at different thickness are presented in Fig. 1 (a), (b), (c) and (d) with diffraction angle 2θ from 20° to 50° . The observed (d) spacing and the respective prominent peaks correspond to reflections at (002) and (103) planes which coincide well with JCPDS data as shown in Table 1. A sharp peak is observed almost in all films close to $2\theta = 25.3^\circ$ corresponding to (002) plane of the hexagonal phase. Another peak commonly observed is at about $2\theta = 45.6^\circ$ with broad and low intensity corresponding to (103) plane of hexagonal structure.

When the thickness is increased, the films became highly oriented along (002) direction and the other peaks are greatly suppressed. Therefore it has been concluded that the deposited CdSe thin films are polycrystalline in

nature with hexagonal structure. Fig. 2 shows the relation between (d) spacing and thickness.

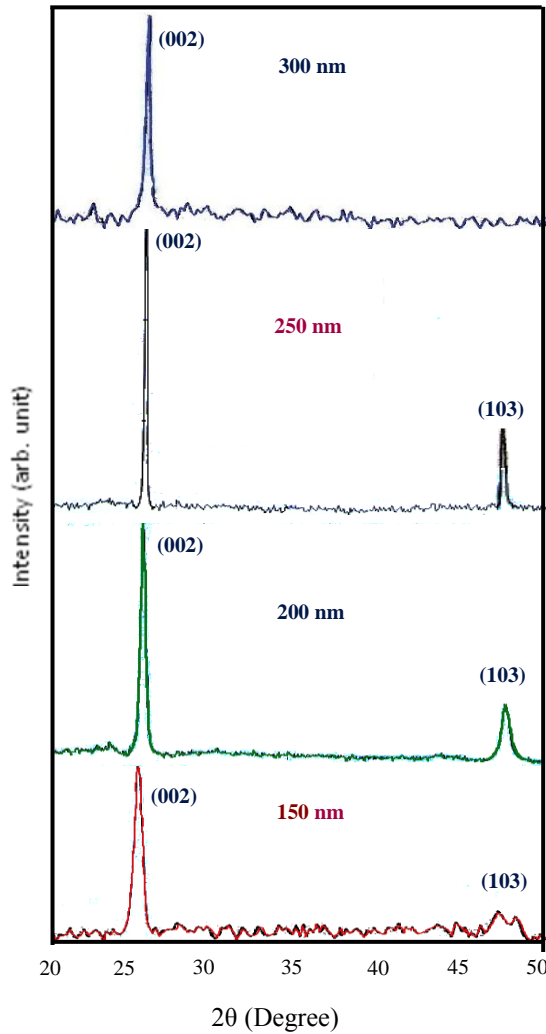


Fig. 1. X-Ray diffraction patterns for CdSe thin films deposited at different thickness.

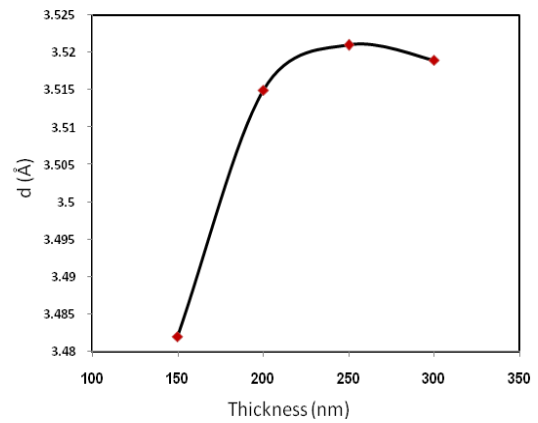


Fig. 2. Relation between d spacing and thickness of CdSe thin films.

The results obtained from XRD show that the FWHM of CdSe films are reduced, which means that the grain size and crystallite of the CdSe films are increased. The result is listed in Table 1 for all samples deposited at different thickness. Fig. 3 shows the effect of thickness on FWHM of CdSe thin films.

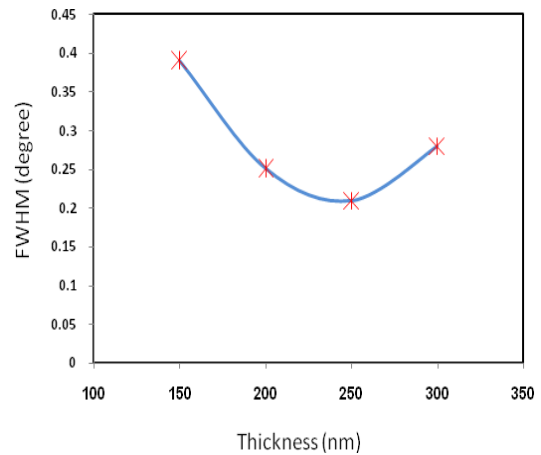


Fig. 3. The relation between thickness and structure FWHM.

Table 1. XRD patterns characteristics of CdSe films at various thicknesses.

Deposition condition	002				103			
	2θ (degree)	I/I_o	d (Å)	β (XRD) (degree)	2θ (degree)	d (Å)	I/I_o	β (XRD) (degree)
ASTM	25.354	70	3.510	-	45.788	1.980	70	-
150 nm	25.362	60	3.482	0.39	45.683	1.853	4	0.37
200 nm	25.409	85	3.515	0.25	45.666	1.858	20	0.35
250 nm	25.286	100	3.521	0.21	45.721	1.904	35	0.23
300 nm	25.328	72	3.519	0.28	-	-	-	-

The lattice parameter (a) is determined for hexagonal structure by the following expression [1]:

$$\frac{1}{d^2} = \frac{4(h^2 + hk + k^2)}{3a^2} + \frac{l^2}{c^2} \quad (1)$$

Where h , k , l are the Miller indices of the lattice plane.

The values of lattice constants for CdSe films deposited at different thickness have been listed in Table 2. It is inferred that the lattice parameters values are in very close agreement with the standard values.

Table 2. Lattice constants as a function of thickness of CdSe thin film.

Deposition condition	investigated line	Lattice (a) Å	Lattice (c) Å
150 nm	002	4.270	6.964
200 nm	002	4.311	7.03
250 nm	002	4.318	7.042
300 nm	002	4.316	7.038
ASTM	002	4.299	7.010

Fig. 4. Shows the dependence of the (002) plane intensity peak on thickness of CdSe thin films.

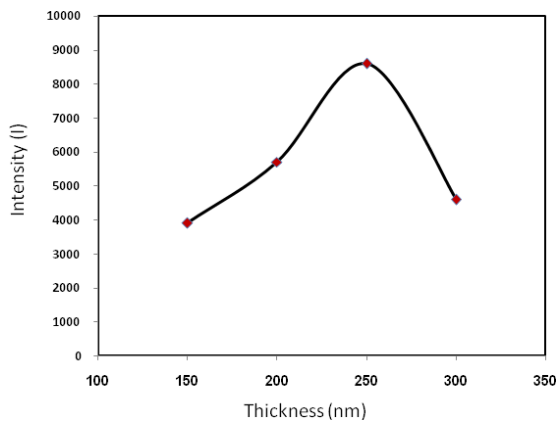


Fig. 4. Effect of thickness on the relative intensity of investigated peak (111).

The grain size (D) is calculated using the Scherrer formula from the full-width half-maximum (FWHM) (β) [10]:

$$D = \frac{k\lambda}{\beta \cos \theta} \quad (2)$$

Where λ is the wavelength of the X-ray used, β is the FWHM, D is the particle size value and θ is half the angle between incident and the scattered X-ray beams. The (D) values listed in the Table 3. It shows that grain size of the films is increased with increasing thickness. The intense and sharp peaks in XRD pattern reveal the good

crystallinity of the films and also confirm the stoichiometric nature of CdSe films as shown in Fig. (5).

Assumes the world Warren that the mathematical representation of curves resulting from the X-ray diffraction (XRD) depends primarily on the amount of similarity between these curves and functions of each of the Cauchy and Gauss. In the case considered X-ray diffraction curve is similar to Cauchy function and take the form of $(1+k^2x^2)^{-1}$, the correction is given by the following relationship, which was called (Scherer's correction):

$$\beta_{cs} = \beta_m - \beta_i \quad (3)$$

Compensation equation (3) in the relationship (2) we get:

$$D = K\lambda / [(\beta_m - \beta_i) \cos(\theta)] \quad (4)$$

In the case considered X-ray diffraction curve similar to the Gauss function which takes the form $\exp(-k^2x^2)$ the accuracy to be higher because of the great similarity between this function and the diffraction curves; it was suggested (Warren) correction form:

$$\beta_{cs}^2 = \beta_m^2 - \beta_i^2 \quad (5)$$

This correction called (Warren's Correction)

Compensation equation (5) in the relationship (2) we get:

$$D = K\lambda / [(\beta_m^2 - \beta_i^2)^{1/2} \cos(\theta)] \quad (6)$$

Since the output line shape does not resemble the Gauss curve and Cauchy curve completely, so these relations have limited operation values. If the intensity curve does not sharp may be used (Scherer's correction) or (Warren's Correction) former because the difference between the values given by relations (4) and (6) is not large, which means that the decrease of the curve breadth (an increase of sharpness) means that the effect of the amount (β_i) is significant, since the width of the curve in the half intensity (FWHM) is inversely proportional with grain size according to equation (2), the decrease in (FWHM) leads to increase in the grain size, which means that few crystal defects are present in the sample.

Moreover, Warren was suggested a relationship takes into account the geometric meaning which is [11, 12]:

$$\beta_{cs} = [(\beta_m - \beta_i)(\beta_m^2 - \beta_i^2)^{1/2}]^{1/2} \quad (7)$$

Compensation equation (7) in the relationship (2) we get:

$$D = K\lambda / [[(\beta_m - \beta_i)(\beta_m^2 - \beta_i^2)^{1/2}]^{1/2} \cos(\theta)] \quad (8)$$

Table 3. Grain size of CdSe thin film.

Deposition condition	investigated line	Grain Size (D) nm eq.(2)	Grain Size (D) nm eq. (4)	Grain Size (D) nm eq. (6)	Grain Size (D) nm eq. (8)
150 nm	002	21.8184	30.3975	22.7502	26.2957
200 nm	002	34.0402	60.7862	37.9240	48.0137
250 nm	002	40.5158	85.0832	47.6007	63.6624
300 nm	002	30.3900	50.0698	33.0476	40.6940

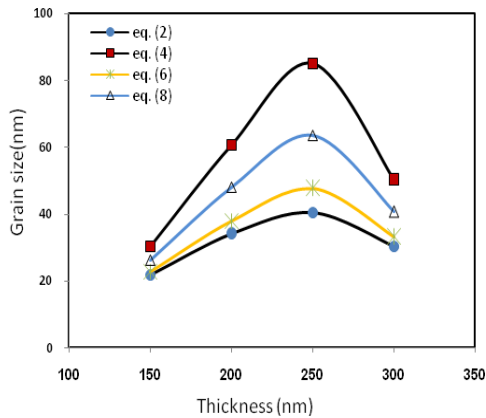


Fig. 5. Grain size as a function of thickness for CdSe thin films.

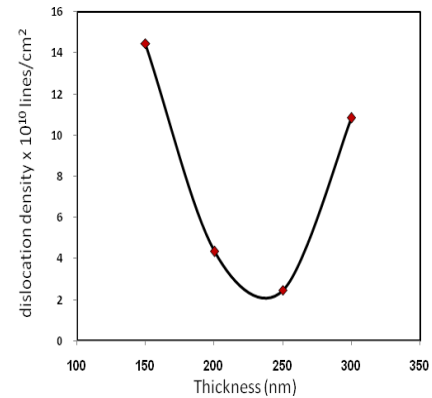


Fig. 6. Dislocation density as a function of thickness for CdSe thin films.

The dislocation density (δ) has been calculated by using the following formula [13], for CdSe thin films:

$$\delta = 1/D^2 \quad (9)$$

The dislocation density for CdSe film is decreased with increasing thickness. It appears clearly from the results that these are an enhancement in the film structure and homogeneous with increasing the thickness up to (250 nm).

Fig. 6 shows the effect of vibration thickness on the value of dislocation density.

The strain values (ϵ) can be evaluated by using the following relation [5]:

$$\epsilon = \beta \cos \theta / 4 \quad (10)$$

It can be generally observed that strain and dislocation density of the film decreases as the particle size increases which is a well-known phenomenon [14]. Strain is inherent and natural component of CdSe materials as shown in Fig. 7. Due to the large number of grain boundaries and the concomitant short distance between them. Moreover, the increasing surface energy contributes to the varying magnitude of strain. Similar results have been observed with increase of thickness for vacuum evaporated CdSe films.

Table 4. Structural parameters of CdSe thin film.

Deposition condition	Grain Size (D) nm eq. (8)	investigated line	Intensity arb. unit	Micro strain (ϵ) $\times 10^{-3}$	density (δ) $\times 10^{10}$ lines/cm ²	Integral breadth (Δ) degree	Shape factor (Φ)
150 nm	26.2957	002	3900	1.6593	14.4620	0.4366	1.1194
200 nm	48.0137	002	5700	1.0635	4.3378	0.1689	0.6756
250 nm	63.6624	002	8600	0.8935	2.4673	0.1131	0.5385
300 nm	30.3900	002	4600	1.1913	10.8277	0.3043	1.0867

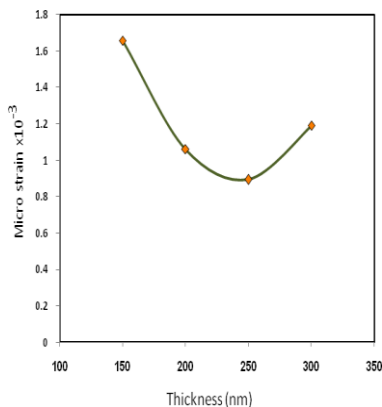


Fig. 7. Micro strain as a function of thickness for CdSe thin films.

Integral breadth (Δ):

There are two branches of line profile analysis:

1. broadening.
2. shape of diffraction line.

The first one is caused by non ideal optics of the instrument, wavelength, dispersion and structural imperfections of the specimen, also this branch is subdivided into size broadening (which is caused by the finite size of domains), and strain broadening (which is caused by varying displacements of the atoms with respect to their reference-lattice positions). The second is frequently characterized by means of one or two breadth measures FWHM, and β which is given by [15]:

$$\Delta = \text{Area} / I_{\max} \quad (11)$$

Where: Area = area under peak.

I_{\max} = maximum intensity.

The shape factor of the line profile resulting from the XRD patterns could be calculated from the relation [15]:

$$\phi = \Delta / \beta \quad (12)$$

All these parameters are calculated and presented in Table 4.

4. Conclusions

CdSe thin films were deposited onto glass substrate by thermal evaporation technique at different thickness. The structures of the films consist of fine (26–40 nm average size) highly oriented grains with hexagonal (002) planes. The grain size increases when the thickness increases. All the films deposited at different thickness show hexagonal structure.

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