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ORIGINAL ARTICLE

Structural And Optical Properties Of Thermally Evaporated Cds Thin Films

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Abstract:

Cadmium Sulphide is an important semiconducting material belonging to group II-VI. This compound has been investigated since many years in crystal and thin film forms. In present investigations, Cadmium Sulphide is deposited in thin film form using thermal evaporation at pressure better than 10-5 torr. The structural and optical characterizations of CdS have been discussed in this paper for three different thicknesses. From the structural characterization (Using XRD technique), it was observed that CdS possesses cubic structure with grain size around 20 nm. The micro strain (ε) and dislocation density (ρ) were also estimated in present case and found to be in the range 16.25x104 – 22.73 x104 lines-m2 and 19x10-5 – 33x10-5 lines/m2 respectively. The lattice parameter was found to be around 5.811? .From the optical characterization, the bandgap of CdS was evaluated and found to vary from 2.46eV to 2.40eV with thickness in the range 6k? - 10k?. In addition to this, the transmission properties were observed to become less effective as the thickness of films increases. The extinction coefficient was found to decrease with increase in thickness of the films..

KEYWORDS:

Cadmium Sulphide, Thin films, Thickness depentent parameters, Structural properties, Optical properties.

1.INTRODUCTION

Group II-VI semiconductors have proved their potential in various optoelectronic applications. These compounds have been investigated both in crystal and thin film form. Many techniques have been used for the deposition of CdS thin films. These include thermal evaporation [1], sputtering [2], chemical bath deposition [3], spray pyrolysis [4], metal organic chemical vapour deposition (MOCVD) [5], molecular beam epitaxy [6], electro deposition [7], photochemical deposition [8] etc. In present investigations, the CdS thin films have been deposited using the thermal evaporation technique. Here CdS thin films of different thicknesses (deposited at pressures better than 10-5 torr) have been investigated for their structural and optical characterizations. It has been seen that CdS can exist in hexagonal or cubic structure. In literature, the presence of hexagonal structure and cubic structure has been found in CdS when investigated in thin film form [9-14]. In present paper the authors report their investigations on the

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structural characterization of CdS and the effect of thickness of films on it. Also, the effect of thickness on optical parameters like band gap, transmittance, extinction coefficient etc. has been discussed in detail in this paper.

2.EXPERIMANTAL

CdS films of 6 k?, 8 k? and 10 k? thicknesse were thermally evaporated and deposited on chemically and ultrasonically cleaned glass substrates with the help of vacuum coating unit (12A4D, HHV). All the gadgets of the vacuum chamber were first cleaned by acetone. A clean evaporation source (molybdenum boat) was fixed in the filament holder inside the chamber. CdS powder having purity 99.99% was kept in the molybdenum boat. The glass substrate was cleaned by acetone and ultrasonic vibrations. The substrate was kept on the substrate holder and crystal monitor was placed near it to measure the thickness during deposition process. The chamber was evacuated at a pressure better than 10-5 torr by the combination of rotary and diffusion pump.When vacuum of 10 -6 torr was attained in the vacuum chamber, the temperature of the boat was gradually raised to heat CdS to temperature greater than the melting point.This allowed the evaporation of CdS material. The X-ray diffraction analysis of CdS films has been carried out at 300K using Philips X-ray diffrectomer, (model: X'PERT MPD Netherland) with CuKα radiation of wave length 1.54 Å.The optical characterization of CdS films were carried out using the UV-VIS-NIR spectrophotometer (Perkin Elmer-USA, Model: Lambda 19) in the range of 200nm to 3200nm wavelength.

3.RESULTS AND DISCUSSIONS

3.1 Structural Properties

The structural characterization of thermally evaporated CdS thin films of different thicknesses has been carried out using X-ray diffraction technique. The XRD patterns of CdS films of thicknesses 6kÅ, 8kÅ, and 10kÅ deposited at substrate temperature 300K are shown in figure 1(a, b and c).

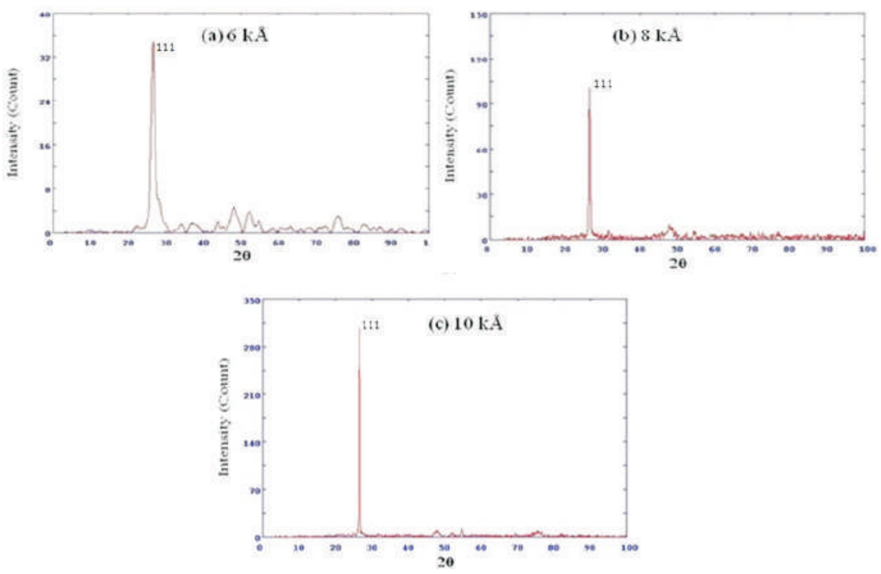

Fig. 1(a, b and c) – X-ray diffraction spectra of Cadmium Sulfide films.

From these XRD patterns, it is quite apprarent that a strong peak with high intensity is observed around 2θ=26.5. It indicates that this angle represents the preferred orientation for the growth of films. All the peaks shown in figure 1 have been assigned the indices. Ultimately, (1 1 1) plane is found to correspond to 26.5 degree of 2θ value which is a preferred orientation. In present investigations, the lattice spacings were calculated for all the three thicknesses using data of XRD and are shown in table 1. The data presented in table 1 show that the results observed in present investigations match with the standard data seen in JCPDS [15] for cubic structure of CdS. It reveals the fact that CdS deposited in thin film form in present case possesses cubic structure.

Table 1 Comparison of structural parameter of CdS thin films.

Thickness	h k l	d-spacing		Grain size D (nm)	Micro strain ε 10^{-4} (lines-m^2)	Dislocation density ρ 10^5 (lines/m^2)	Lattice constant a=b=c (?)
		XRD	JCPDS				
6 k?	1 1 1	3.358	3.359	17.24	22.73	33	5.811
8 k?	1 1 1	3.357	3.359	20.83	17.74	23	5.814
10 k?	1 1 1	3.355	3.360	22.45	16.25	19	5.816

The lattice constant 'a' for all the thicknesses of CdS thin films has been calculated using the following formula [16].

$$\frac{1}{d^2} \pi \frac{h^2 \pi k^2 \pi l^2}{a^2} \qquad (1)$$

The efforts were made to calculate the grain size of CdS in all the films deposited in present case with the help of data obtain from the XRD and Debye-Scherer's relation given in equation (2)[16].

$$D \pi \frac{k\pi}{\pi \cos\pi} \qquad (2)$$

Where
k is the constant = 0.94, l.
λ- the wavelength of radiation.
β - The full width half maximum and θ – the diffraction angle.

The micro strain (ε) and the dislocation density () of the deposited films were evaluated using the equations (3) and (4) given below.

$$\pi \pi \frac{\pi \cos\pi}{4} \qquad (3)$$

and

$$\pi \pi \frac{1}{D^2} \qquad (4)$$

The results of these calculations have also been presented in table 1. It was found that there is an increase in the grain size as the thickness of the films increases [17, 18]. Some of the parameters like particle size (D) , strain (ε), dislocation density (ρ) and lattice constant have also been calculated using the same data and are given in table 1. The data presented in table 1 match with the earlier reports. [17, 18].

3.2 Optical properties

The optical absorption and transmittance measurements of all the three CdS thin films have been carried out at room temperature. The optical spectra of thermally evaporated CdS thin films have been recorded in the wavelength range from 200nm to 3200nm. The results of these investigations have been used for the calculations of the absorption coefficient and other parameters. To confirm the direct or indirect nature of the optical transitions of carriers in all the three CdS thin films, the above calculated absorption coefficient corresponding to each energy of incident radiation has been plotted with respect to the energy of the incident photons. The intercepts of the straight lines drawn from the linear portion of $(\alpha h\nu)2$ vs. $(h\nu)$ for all the thicknesses are shown in fig.2 and they have been used to evaluate the band gap energies in CdS in present case. The values of direct band gap observed here are given in table 2 for CdS thin films which are in good agreement with the reported data[17].

From this table, it is quite clear that the value of direct band gap in CdS films decreases with increase in thickness in present investigations. Similar results can be seen in literature for CdS compound [18]. It is interesting to note that the variation of band gap with thickness of different semiconductors belonging to group II-VI have been studied by various workers [10, 19-23]. In some compounds, like ZnTe, the band gap is found to decrease with increase in thickness same as in CdS. In present investigations, the existence of only direct band gap is conformed which is responsible for the allowed transitions from valance band to conduction band.

Using the data of absorption spectra, the transmittances were calculated for CdS thin films for all the thicknesses and have been shown in figure 3. From these spectra, it can be clearly seen that CdS is not transparent for the wave length below 500 nm. Above this wave length the percentage of transmittance arises rapidly. This is an obvious fact due to the high values of the band gap of CdS. Also, similar results can be found in literature for CdS compound [18]. The efforts have been made to study the absorption losses in CdS in thin film form for present investigations. For this purpose, the data derived from optical characterizations have been discussed above.

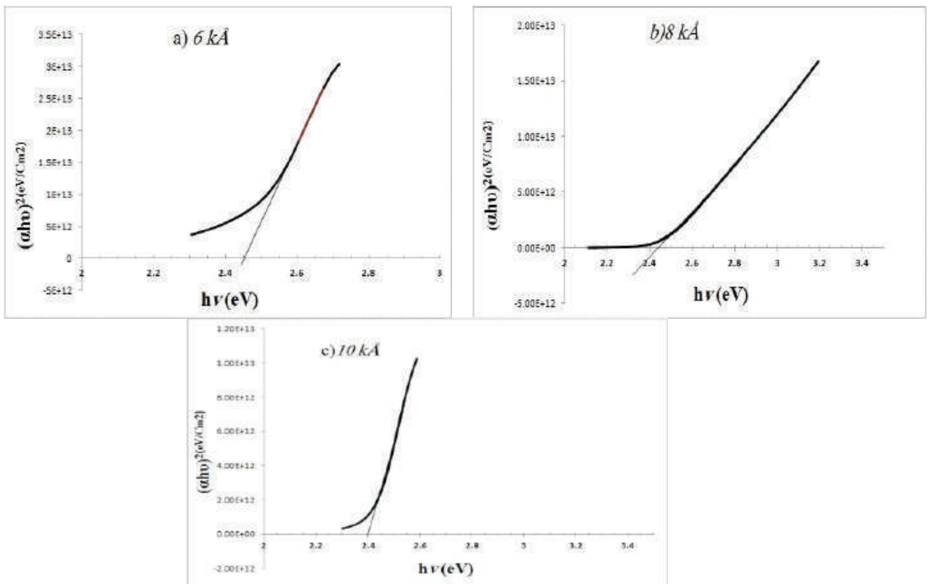

Fig. 2 (a, b and c) – Plots of $(\alpha h\upsilon)2$ vs $h\upsilon$ for CdS films of different thicknesses.

Table 2. Band gap of CdS films at different thicknesses

Thickness	Band gap
6 k?	2.46 eV
8 k?	2.45 eV
10 k?	2.40 eV

In light of this, the extinction coefficient was estimated for all the three thicknesses of CdS films. The extinction coefficient can be given by the relation [19].

$$K \pi \frac{\pi \pi}{4\pi} \qquad (6)$$

Where α is the absorption coefficient which may be written as 2.303A/t. Here A is absorbance and t is the thickness of the film.

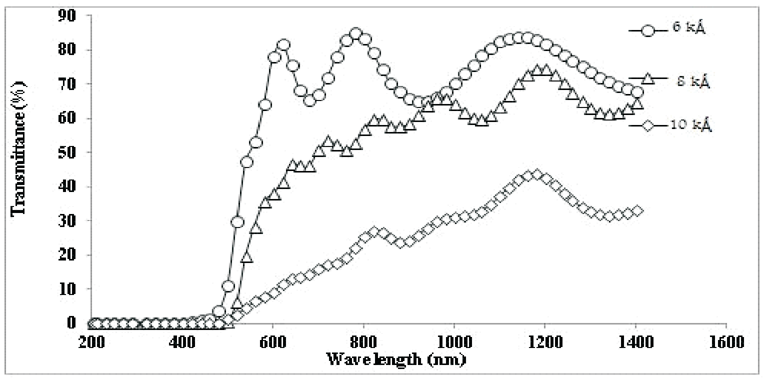

Fig. 3 Transmittance spectra of CdS films.

Using the same relation, the variation of extinction coefficient with wavelength was also evaluated in present case. These results have been graphically presented in figure 4. From figure 4, it is quite apparent that as one moves from ultraviolet to visible region, irregular increase in extinction coefficient k is observed. This increase is followed by sudden decreased at around 500nm which lies in visible region. However, with increase in film thickness, it is observed that extinction coefficient relatively decreases at all wavelengths.

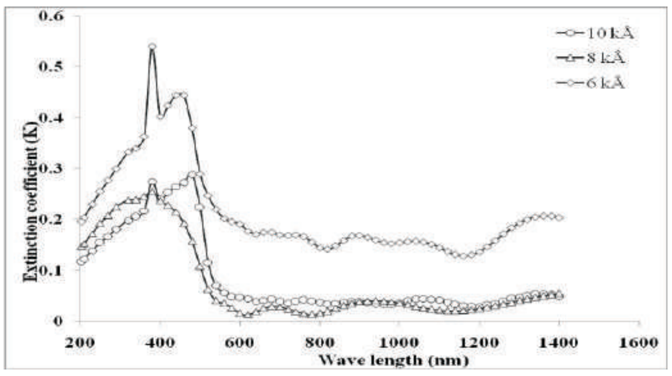

Fig 4. The variation of extinction coefficient with wavelength for CdS thin films.

4.CONCLUSION

From the structural characterizations of CdS thin films in present investigations, it was confirmed that the cubic structure exists with preferred orientation at 2θ = 26.5°. The grain size was observed to increase with increase in thicknesses. From the optical characterizations, it was inferred that the band gap of CdS in present case was varying from 2.46eV to 2.40eV for thicknesses of CdS thin films ranging from 6 k? to 10 k?. Also, it was found that below 500 nm wave lengths, CdS exhibits very low transmission characteristics. Cadmium Sulfide is found to have highly absorption behavior in visible range of wave length. Besides this, the transmission properties are observed to decreases as the thickness of the films increases. In addition to this, the extinction coefficient increases with decrease in thickness.

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