Journal of Ovonic Research Vol. 7, No. 4, July – August 2011, p. 83 - 92

STRUCTURAL, ELECTRICAL AND OPTICAL PROPERTIES OF CdS THIN FILMS BY VACUUM EVAPORATION DEPOSITION

D. KATHIRVEL[a*], N. SURIYANARAYANAN [b], S. PRABAHAR [c], S. SRIKANTH [c]
[a]*Department of Physics, Kalaignar Karunanidhi Institute of Technology, Coimbatore, India*
[b]*Department of Physics, Government College of Technology, Coimbatore, India.*
cDepartment of Physics, Tamilnadu College of Engineering, Coimbatore, India

Cadmium Sulphide thin films have been deposited on to well cleaned glass substrate in a vacuum of 10^{-6} Torr. The thickness of the films has been determined by quartz crystal monitor method. CdS thin film of lower thicknesses has amorphous structure and higher thickness has polycrystalline nature with cubic structure. The structural parameters such as interplannar distance (d), lattice constant (a), grain size (D), dislocation density and microstrain have been evaluated. The optical properties have been studied in the range of wavelength 300-900nm. It is observed that band gap energy is inversely depended on film thickness. The electrical resistivity measurements were performed at room temperature by four probe method and it shows CdS films with high ressitivity.

(Received July 22, 2011; accepted August 29, 2011)

Keywords: CdS, Structural Properties, X-ray diffraction, Electrical Properties

1. Introduction

The wide energy gap of CdS semiconductor is one of the most important properties leading to the great experimental interest in these materials. CdS is a suitable window layer for solar cells [1-3] and also finds applications as optical filters and multilayer light emitting diodes [2], photo detectors [3], TFETs [3-5], gas sensors [6] and transparent conducting semiconductors for optoelectronic devices [7]. Various methods are used to deposit CdS thin films [8-13]. Among the vacuum evaporation is a attractive, effective method and the application at enables the deposition of thin films of larger area with good uniformity. The present study reveals the variation of structural, optical and electrical properties of CdS thin films.

2. Experimental methods

Using the conventional 12A4 hind highvac coating unit pure (99.999%) aluminium was evaporated from tungsten filament on to well cleaned glass substrates through suitable masks to form to the base electrodes. Pure (99.99%) CdS (Alrich chemicals company, USA) was then evaporated from molybdenum boat to form the dielectric layer. A working pressure of 10^{-6} Torr was maintained in all the evaporation processes. For the optical and structural analysis, the CdS thin films were deposited on the glass substrates.

---

[*]Corresponding author: kathirvelde.41@gmail.com

3. Results and discussion

3.1 Structural analysis of CdS thin films

X-ray diffractogram of CdS thin films, taken from diffractometer is used to analyze various crystalline aspects. According to Bragg's law,

$$n\lambda = 2d_{hkl} \sin Q_{hkl} \tag{1}$$

Where 'n' is the order of reflection, 'λ' is the wavelength of the incident x-rays. The direction of propagation of scattered beams (Q_{hkl}) is related to the interplanar distance (d_{hkl}) in the lattice (h k l) which represents the property of the material and is related with the lattice constant and miller indices[14-15]. The XRD pattern for CdS thin films of thickness 2550 Å, 930 Å and 880 Å are shown in Fig. 1, Fig. 2 and Fig. 3.

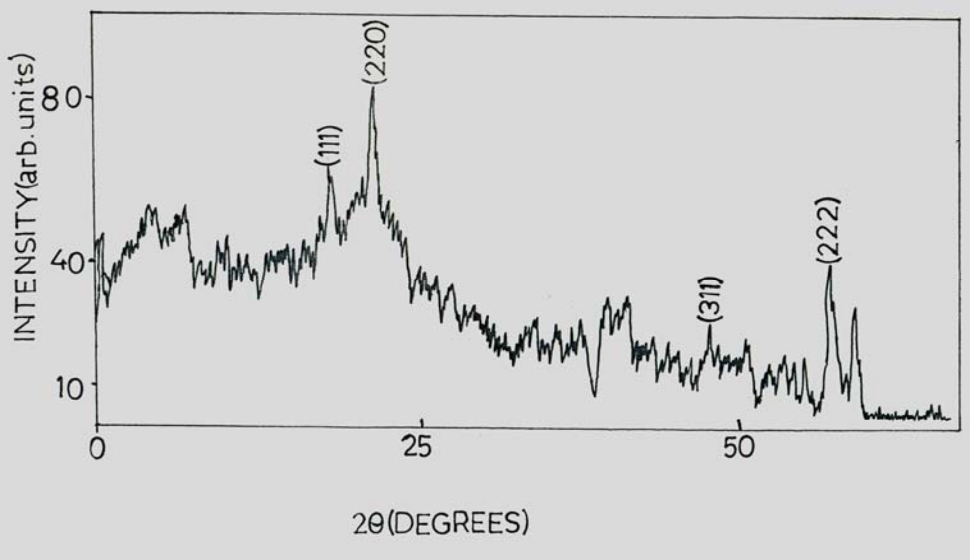

Fig. 1. X-ray diffractogram of CdS thin film of thickness 2550 Å.

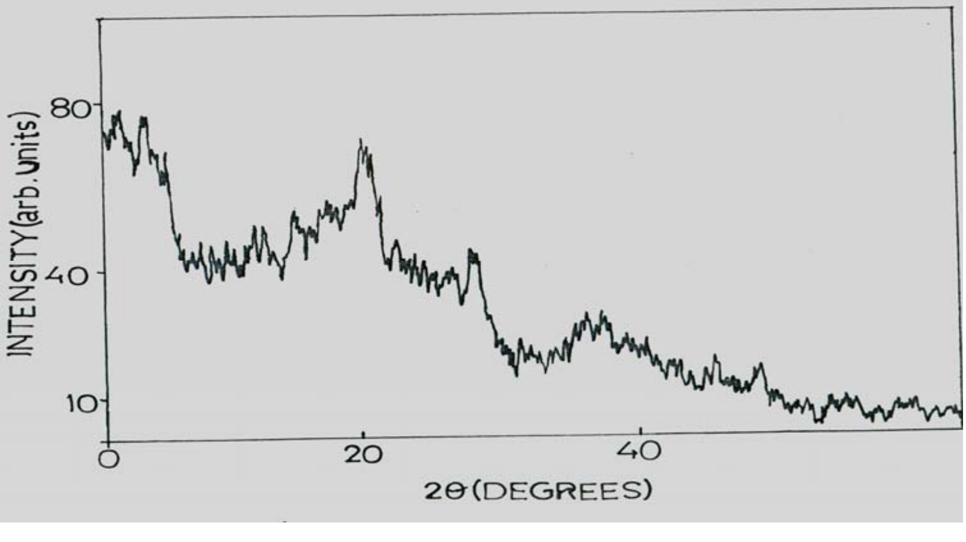

Fig. 2. X-ray diffractogram of CdS thin film of thickness 930 Å

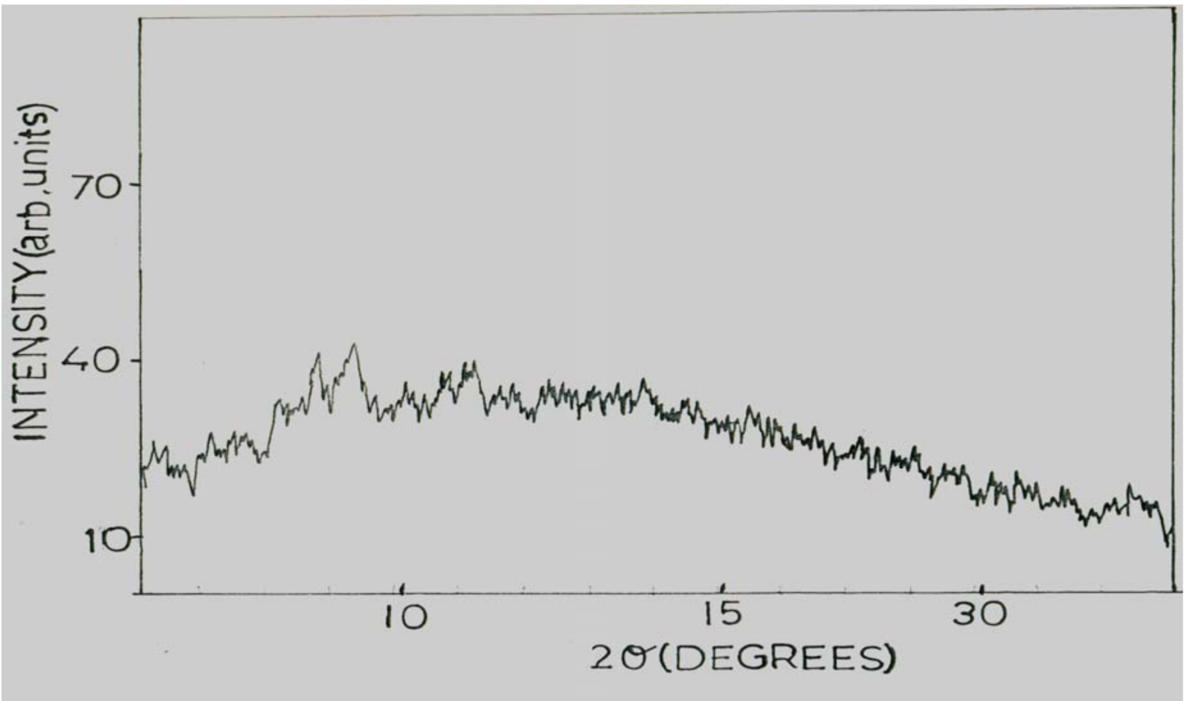

Fig. 3. X-ray diffractogram of CdS thin film of thickness 880 Å

Fig 1. shows that the CdS thin film of thickness 2550 Å has to the presence of peaks confirms the sample is in crystalline form. In the case of the films with lower thickness 930 Å and 880 Å, the observed featureless spectrum in both the films leads as to understand the films are amorphous in structure, and thus confirms the glassy nature of the CdS thin film at lower thickness [16-17].

The inter planar distance (d) and the lattice parameter (a) are calculated in this case by means of the plane-spacing equation for cubic crystal, which is given by,

$$1/d^2 = (h^2+k^2+l^2)/ a^2 \qquad (2)$$

and the grain size is calculated using Scherer's formula,

$$D = K\lambda / \beta \cos \theta \qquad (3)$$

Where 'β' is the full width half maximum of the peaks. The diffraction direction is solely determined by the structure and size of the unit cell. The calculated 'd' values for CdS sample coincides fairly with those of bulk material reported in ASTM tables on cubic CdS. All this crystalline showed clear evidence for a cubic CdS [18]. The interplanar distance (d), lattice parameter (a), grain size (D), dislocation density (ρ) and microstrain (ε) are shown in table 1.

Table 1. Structural parameters for CdS thin films

Thickness	(h k l)	d (Å) Exp	d (Å) ASTM	2 θ	a (Å)	Grain size (D) Å	Dislocation density (ρ)cm^2	Strain (ε) 10^{-3}
2550 Å	222	1.59	1.57	29	5.5079	3.5752	7.3903	9.7021
	311	1.64	1.64	28	5.4392	5.0631	3.7315	6.8512
	220	1.89	1.93	24	5.3598	2.6192	14.4167	13.2406
	111	3.18	3.16	14	5.5079	5.2884	3.3730	6.5516

From the table 1, it is found that, the grain size of the film increases with film thickness and the dislocation density and microstrain are found to decrease. It can be attributed to the decrease in the imperfections and dislocations of the films with increasing film thickness.

3.2 Electrical Properties

The electrical resistivity of CdS films with different thickness was measured using the d.c. four probe method in air. Fig. 4 -6 shows the variation of (log ρ) with reciprocal of temperature (1000/T). For all films, it was seen that resistivity decreases with temperature indicating semiconducting nature of films [19]. For all the films, resistivity follows the relation,

$$\rho = \rho_0 \exp (E_0 /KT) \quad (4)$$

Where 'ρ' is resistivity at temperature 'T', ρ_0 is a constant, 'K' the Boltzmann constant (1.38×10^{-23} J/k) and 'E_0' the activation energy required for conduction. Resistivity of CdS thin film decreases due to the improvement in crystallinity of the films as the film thickness increased. This observation is attributed to the size effect observed in semiconductor thin films.

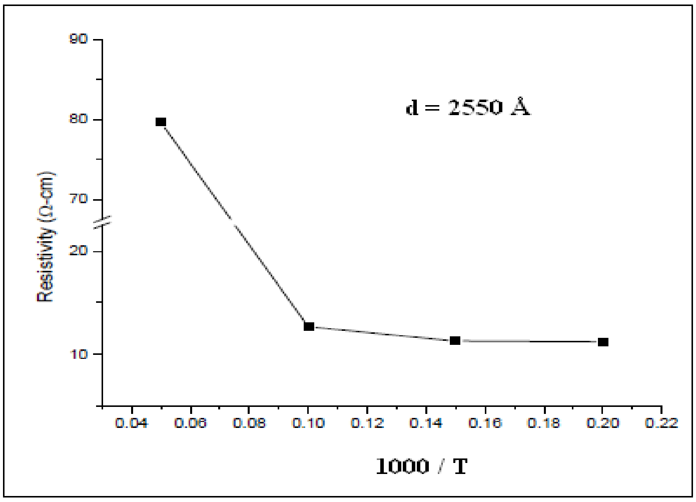

Fig. 4. Resistivity Vs (1000/T) of CdS thin film of thickness 2550 Å

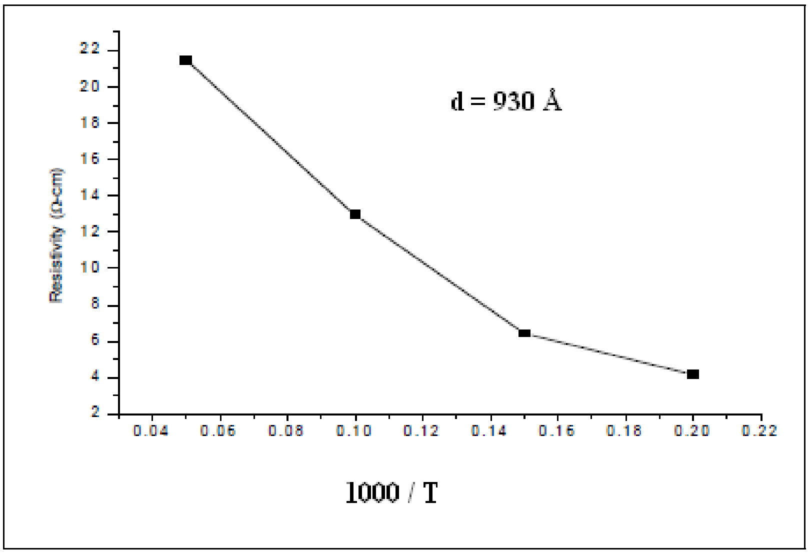

Fig. 5. Resistivity Vs (1000/T) of CdS thin film of thickness 930 Å

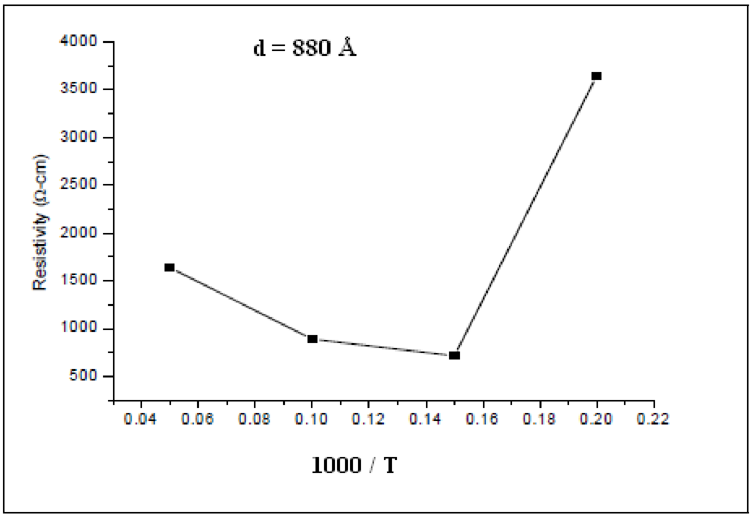

Fig. 6. Resistivity Vs (1000/T) of CdS thin film of thickness 880 Å

From the resistivity plot, the thermal activation energies were calculated using the formula (4). Table 2. Show activation energies at different thickness of CdS film. Activation energies are to the order of 0.7095 to 0.6345 eV as film thickness was decreased from 2550 Å to 880 Å.

Table 2. Variation of activation energy with film thickness

Film thickness (Å)	Activation energy (eV)
2550 Å	0.7095
930 Å	0.6547
880 Å	0.6345

3.3 Optical properties

Transmission spectra of films were recorded as a function of wavelength in the range of 400-900nm. The transmittance spectra of the CdS films in the visible region for the different thickness films are shown in the Fig.7. It reveals that the transmittance decreases with the increase of film thickness.

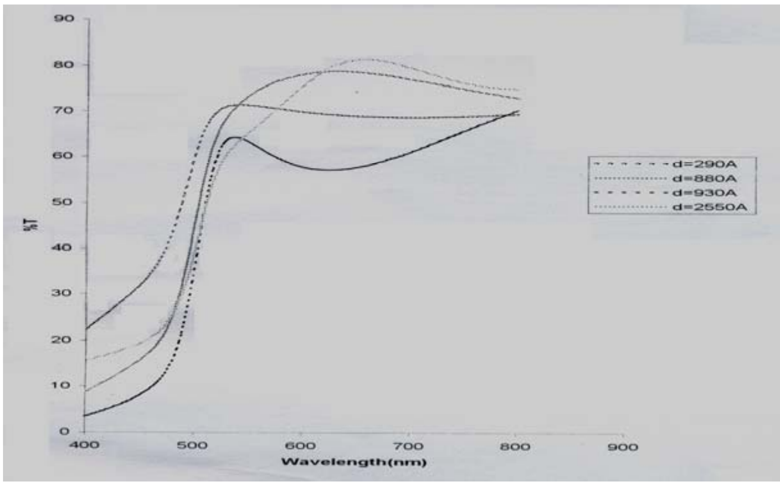

Fig. 7. Transmittance Spectra of CdS thin films for various thickness

From the Fig.8 Optical properties of CdS thin films are determined from absorbance measurements in the range of 300-900nm. The absorption coefficient can be written in terms of the incident radiation energy.

$$\alpha = A\,(h\gamma - Eg) \tag{5}$$

Where 'h' is the Planck's constant and 'γ' is the frequency of the incident radiation.

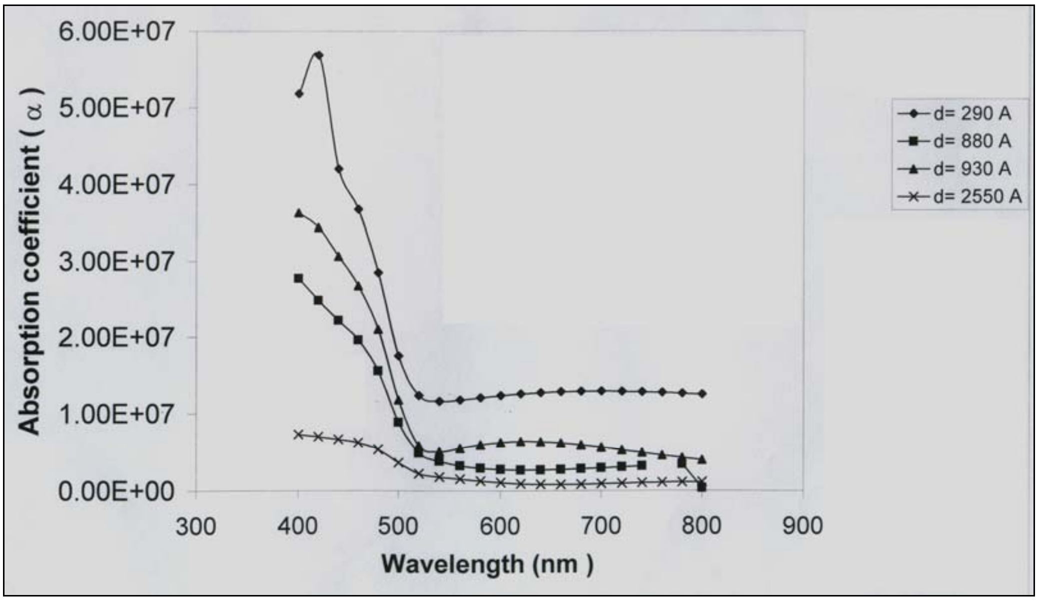

Fig. 7. Absorbance Spectra of CdS thin films for various thickness

From the Fig. 9. the value of Extinction Coefficient (Kf) decreases with the increases in the film thickness. Absorption coefficient (α) associated with the strong absorption region of the films was calculated from absorbance (A) and the film thickness (t) using the relation.

$$A = 2.3026\ A/t \tag{5}$$

The Extinction coefficients are calculated using the equation.

$$K_f = 2.303\ \lambda \log (1/T_0) / 4\pi d \tag{6}$$

The extinction coefficient (K_f) is directly related to the absorption of light. In the case of polycrystalline films, extra absorption of light occurs at the grain boundaries [20]. This leads to non-zero value of (K) for photon energies smaller than the fundamental absorption edge [21].

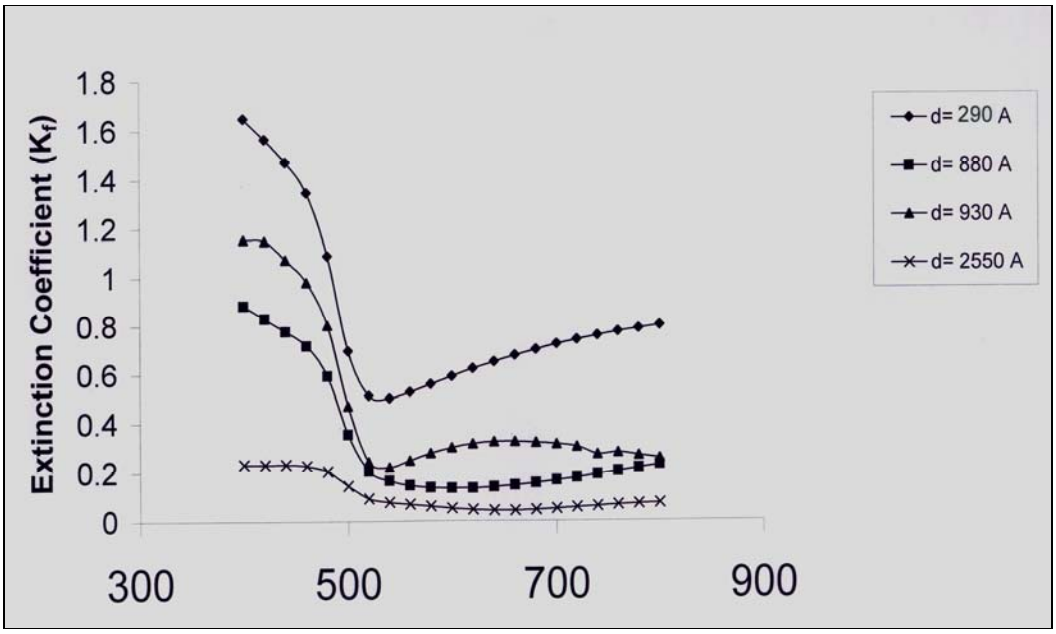

Fig. 9. Thickness dependence of Extinction Coefficient (K_f)

The optical band gab can be obtained by extra plotting the linear portion of the plot $(\alpha h\gamma)^2$ Versus hγ. From the plot, the variation of $(\alpha h\gamma)^2$ Versus photon energy for different thickness (290 Å, 880 Å, 930 Å, 2550 Å) CdS thin films are shown in Fig. 10, 11, 12 and Fig. 13 respectively. The presence of a single slope in the curves suggests that from thermal evaporation are of single phase in nature and the type of transition is direct and allowed [22].

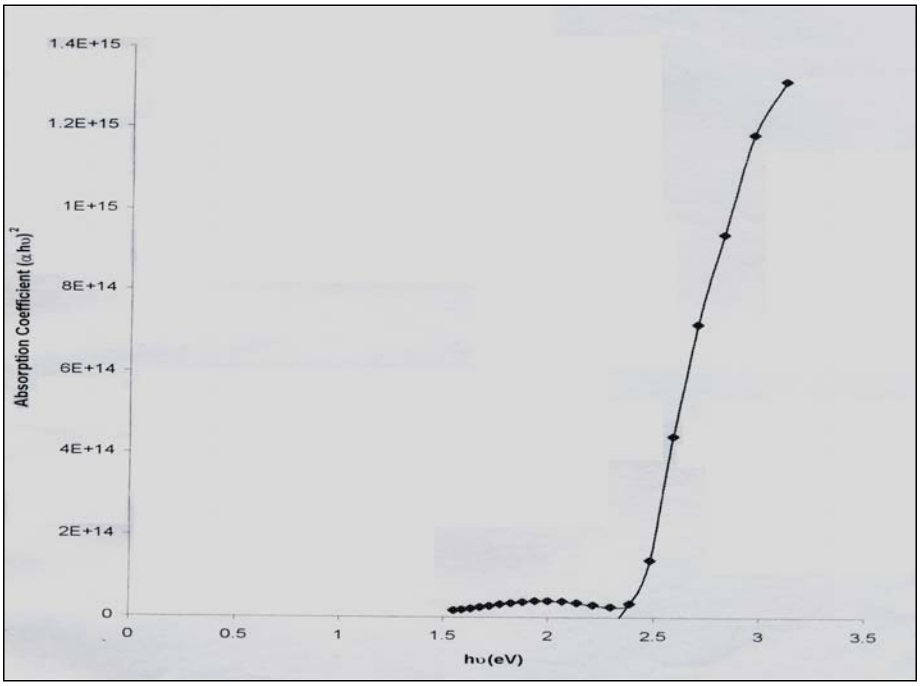

Fig. 10. A plot of $(\alpha h\gamma)^2$ Vs. (hv) for CdS thin film of thickness290Å

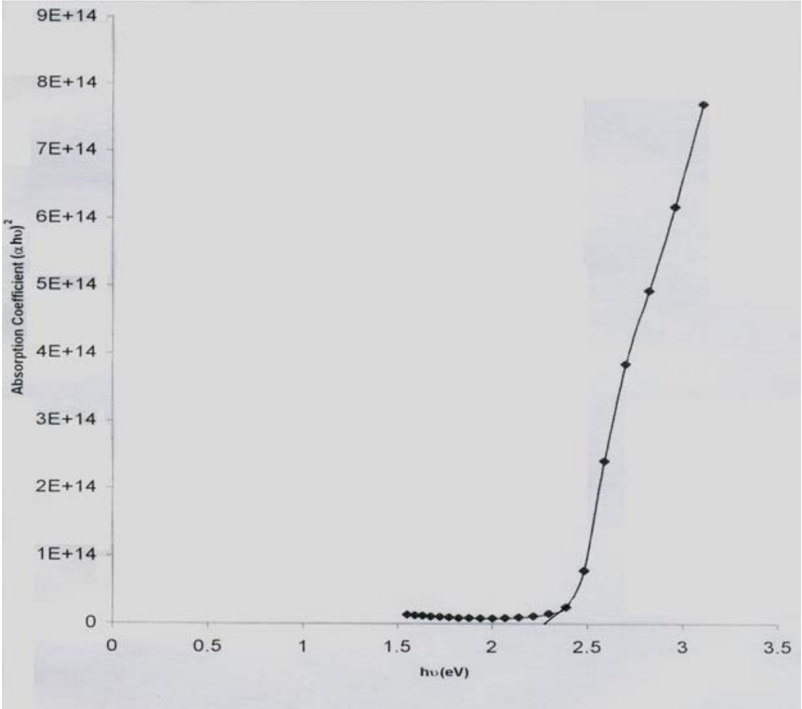

Fig. 11. A plot of (αhγ)^2 Vs. (hν) for CdS thin film of thickness 880 Å

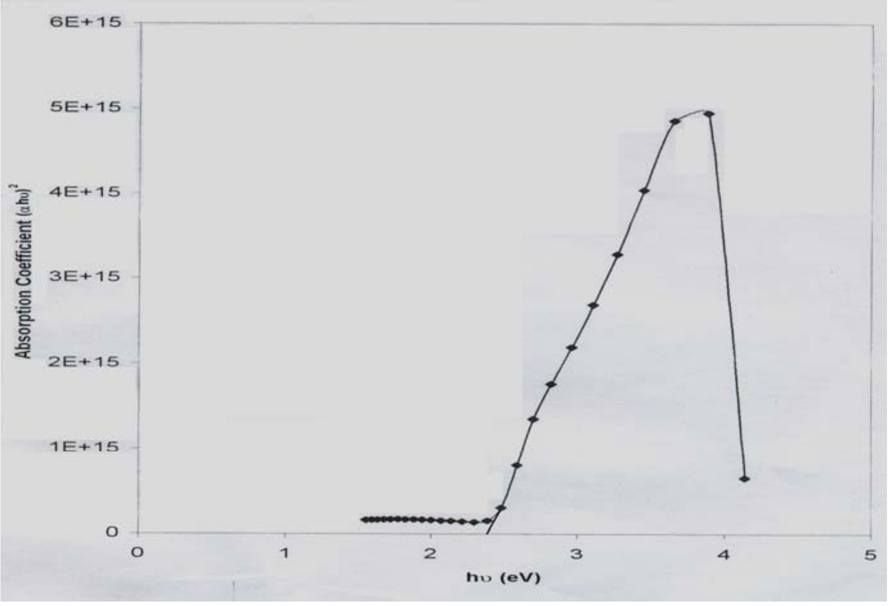

Fig. 12. A plot of (αhγ)^2 Vs. (hν) for CdS thin film of thicknes 930 Å

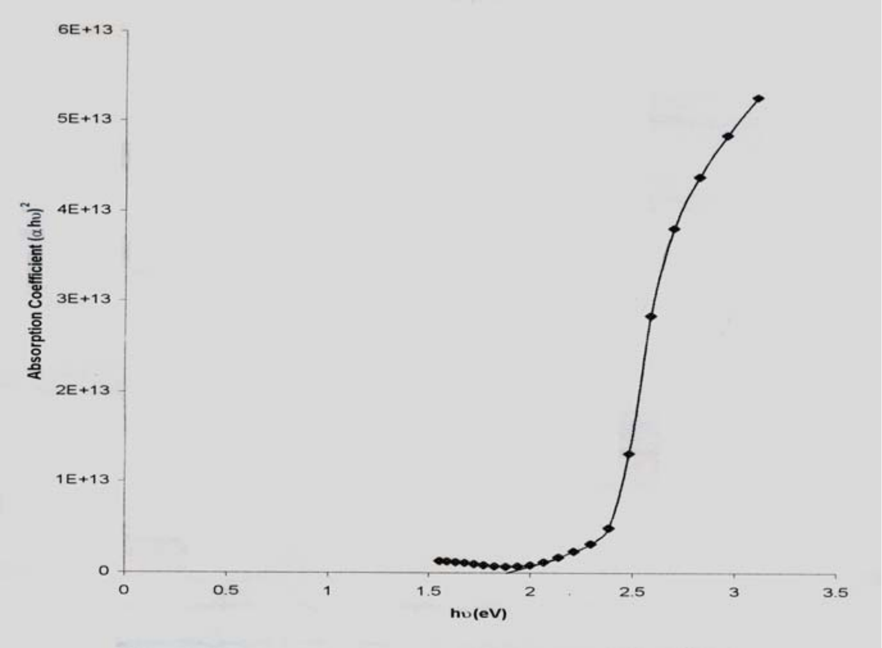

Fig. 13. A plot of $(\alpha h\gamma)^2$ *Vs. (hν) for CdS thin film of thickness 2550 Å*

From these absorption peaks, the direct and allowed band gap energy is evaluated from the plot $(\alpha h\gamma)^2$ Versus hγ are shown in table 3.

Table 3. Variation of energy gap with thickness

Thickness Å	Band gap energy (eV)
290	2.43
880	2.33
930	2.31
2550	1.96

The observed decrease in the band gap energy with increases in thickness is due to the changes in the barrier height to the size of the grain in crystalline film and large density of dislocation.

4. Conclusions

CdS thin films prepared from Vacuum Evaporation deposition are amorphous nature in lower thickness and polycrystalline nature with cubic structure in higher thickness. The transmittance and absorbance spectra in the range of 400-900nm has been taken by using FTIR spectrometer. In absorbance spectra, the material has a high absorbing nature. The observed band gap energy is inversely dependent on film thickness. The electrical resistivity measurements were performed at room temperature by four probe method and it shows CdS films with high resistivity.

References

[1] J.Herrero, M.T.Gutierrez, C.Guillen, J.M.Dona, M.A.Martinez, A.M.Chaparro, R.Bayon, Thin Solid Films **361** 28 (2000).
[2] M.E.Calixto, P.J Sebastian, Solar Energy Materials and Solar Cells **59** 65 (1999).

[3] U.Pal, R.Silva-Gonzalez, G.Martinez-Montes, M.Gracia-Jimenez, M.A.Vidal, Sh.Torres, Thin Solid Films **305** 345 (1997).
[4] J.H. Schon, O.Schenker, B.Batlogg, Thin Solid Films **385** 271 (2001).
[5] J.Levinson, F.R.Shepherd, P.J.Scanlon, W.D.Westwood, G.Este, M.Rider, Journal of Applied Physics **53** 1193 (1982).
[6] Toshiya Hayashi, Takehiro Nishikura, Tatsuro Suzuki, Yoshinori Ema, Journal of Applied Physics **64** 3542 (1988).
[7] T.L.Chu, S.S.Chu, C.Ferekides, C.Q.Wu, J.Britt, C.Wang, Journal of Applied Physics **70** 7608 (1991).
[8] T.L.Chu, S.S. Chu, C. Ferekides, C.Q. Wu, J. Britt, C. Wang, J. Appl. Phys **70** 608 (1991).
[9] S. Mathew, P.S. Mukerjee, K.P. Vijayakumar, Thin Solid Films **254** 278 (1995).
[10] S.J. Castilo, A. Mendoza-Galvan, R. Ramirez-Bon, F.J. Espinoza-Beltran, M. Sotelo-Lerma, J. Gonzalez-Hernandez, G. Martinez, Thin Solid Films **373** 10 (2000).
[11] G.C. Mories, R. Vanderveen, Sol. Energy Mater. Sol. Cells **27** 305 (1992).
[12] B. Ullrich, H. Sakai, Y. Segawa, Thin Solid Films **385** 220 (2001).
[13] H. Ashour, F. El Akkad, Phy. Status Solidi (a) **184** 175 (2001).
[14] Shailaja kolhe, S.K Kulkarni, M.G.Takwale, V.G. Bhide, Sol.Energy Mater. **13** 203 (1986).
[15] D.P.Amalnerkar, K.Yamaguchi, T.Kajita, H.Minoura, Solid State Commun. **90** 3(1994).
[16] B.Ulrich, H.Sakai, Y.Segawa, Thin Solid Films **385** 220 (1992).
[17] P. N.Gibson, M. E. Ozsan, D. Lincot, P. Cowache, D.Summa, Thin Solid Films **361-362,** 34 (2000).
[18] S. Prabahar, M. Dhanam, J. Crystal growth **285** 41 (2005).
[19] S. Prabahar, N. Surynarayanan, S. Srikanth, D. Kathirvel Chalcogenide Letters **6** 309 (2009).
[20] V. Damodara Das, K.Seetharama Bhat, J. Material Science-Materials in Electronics **1** 169 (1990).
[21] T. Mahalingam, M.Radhakrishnan, C.Balasubramaniam, Thin Solid Films **78 (3)** 299 (1981).
[22] H.Metin, R.Esen, Semicond.Sci.Technol, **18** 647 (2003).