

## Synthesis and Characterization of Nanocrystalline (CdS)<sub>0.6</sub>Te<sub>0.4</sub> Thin Films Deposited by Closed Space Sublimation Technique

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**Abstract:** The ternary alloy of (CdS)<sub>0.6</sub>Te<sub>0.4</sub> thin films were deposited onto rotating amorphous glass substrates by using closed space sublimation, at a base pressure of 10<sup>-5</sup> torr. The crystalline, morphological, optical and transport properties of the deposited films were studied by using X-Ray Diffraction (XRD), Scanning Electron Microscopy (SEM), UV-VIS-NIR Spectrophotometer, Four Probe method and Thermo Electric Power (TEP) measurement. The XRD exhibits the deposited thin film has polycrystalline nature having monoclinic phase. The dislocation density ( $\delta$ ), strain ( $\epsilon$ ) and the number of crystallites per unit area ( $N$ ) have been found to be  $2.047 \times 10^{14}$  lines / cm<sup>2</sup>, 0.9926 and  $9.264 \times 10^{17}$  respectively. The SEM reveals the homogeneity of the deposited samples. Optical study performed to estimate optical band gap using absorbance spectra and found to be in the range of 1.6 – 2.1 eV. The four probe method estimates the Electrical Resistivity = 0.2045  $\Omega$ -cm and Activation Energy = 0.01822 eV. The Fermi energy = 0.2628 eV and Scattering Coefficient = 2.3188 evaluated by using TEP.

**Keywords:** Closed Space Sublimation, XRD, SEM, UV-VIS-NIR, TEP.

### I. INTRODUCTION

Many researcher works on binary and ternary alloy of II-VI group elements. CdS and CdTe are promising materials in the fabrication of photo voltaic devices, because of their optical band gap lies within the range of 1-3 eV [1, 2]. The polycrystalline CdS is commonly used for window material. The device performance gets reduced because of two issues. First, it has the absorption within in a short wavelength region due to its band gap of 2.4 eV. Second, inter diffusion along with the absorber layer and window layer [3, 4]. The best way to resolve these problems, find out the material with higher optical band gap than CdS and the inter diffusion can be controlled by depositing a CdS<sub>1-x</sub>Te<sub>x</sub> absorber layer having S content near the solubility limit [5, 6]. The lattice mismatch and interference state can be reduced by incorporation of the CdS<sub>1-x</sub>Te<sub>x</sub> absorber layer in the structure of the CdS/CdTe cells. In CdS<sub>1-x</sub>Te<sub>x</sub> physical properties can be altered by changing the value of x [7]. The parabolic dependence of optical band gap is on the compositions used in alloys [8]. The optical band gap of CdS can be diminished sharply with introducing the Te [9].

There are various techniques are available for the preparation of CdS and CdTe thin film like chemical bath deposition [10], closed space sublimation [11, 12], MOCVD [13], sputtering [14], spray pyrolysis [15], pulse laser deposition [16]. The physical properties of the films can be affected by deposition techniques and deposition parameter. The thin films prepared by vacuum evaporation technique are uniform with excellent crystallinity, dense and highly oriented [17]. The quality and properties of film mainly depend on pressure, deposition rate, substrate temperature and thickness of the film [18].

In this paper we studied the influence of thickness on the structural optical and transport properties of (CdS)<sub>0.6</sub>Te<sub>0.4</sub> thin films, grown by closed space sublimation technique deposited onto rotating amorphous glass substrates.

### II. Experimental

#### 2.1. Preparation of Ternary Compound

The ternary alloy of (CdS)<sub>0.6</sub>Te<sub>0.4</sub> have been prepared by melt quench method. The direct mixture of extremely pure CdS and Te (purity 99.999%), in accordance with their atomic ratio was kept in evacuated quartz ampoule at pressure 10<sup>-5</sup> torr. The ampoule was heated at temperature about 1150 °C for 10 hrs duration. Then the ampoule is quenched in ice cooled water.

#### 2.2. Synthesis of Thin Films

The ternary compound of (CdS)<sub>0.6</sub>Te<sub>0.4</sub> have been deposited onto rotating glass substrate, by closed space sublimation technique, under the pressure of 10<sup>-5</sup> torr. The substrate to source distance was kept at 15 cm. The samples of different thicknesses were deposited under similar conditions. During the synthesis the film thickness was monitored on quartz crystal thickness monitor (DTM-101) provided by Hind-Hi Vac. The deposition rate maintained at 5-8 Å/sec throughout sample preparation. Before evaporation, the glass substrates were cleaned thoroughly using concentrated chromic acid, detergent, distilled water and acetone.

XRD data have been obtained by using x ray Diffractometer (Bruker) within range of 20° - 80° having CuK $\alpha$  radiation. Surface morphological studies of deposited films were done by using the Scanning Electron Microscope (Hitachi, Japan). Optical properties of the samples were estimated by Shimadzu – 2450 Spectrophotometer over the wavelength range of 300 – 900 nm. The resistivity and activation energy of the samples was measured by four probe technique (SES Instruments, Roorkee). The Fermi energy and scattering coefficient was calculated by TEP set up (DMV - 001, Pushpa Scientific, Hyderabad),

### III. Results And Discussion

#### 3.1. Crystalline Analysis

The XRD spectrum of (CdS)<sub>0.6</sub>Te<sub>0.4</sub> thin film having thickness of 1000 Å is shown in Figure 1.

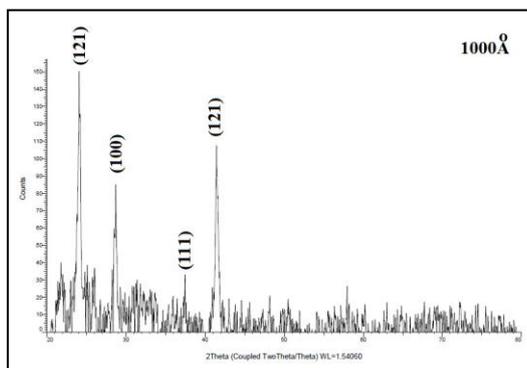


Fig.1. XRD Pattern of (CdS)<sub>0.6</sub>Te<sub>0.4</sub> Thin Film

From X ray diffraction pattern crystalline structure of (CdS)<sub>0.6</sub>Te<sub>0.4</sub> thin film is found to be monoclinic in phase and polycrystalline nature. The XRD spectrum of samples shows the peak 2 $\theta$  at 24.0, 28.8, 37.2, 41.5 having preferred orientation along the (121), (100), (111), (121) plane matches with JCPDS data card 43-0985 and 65-2216. The crystalline size (D) of the sample at 24° was found to be 22.1 nm by using Scherrer's formula:

$$D = \frac{0.9 \lambda}{\beta \cos \theta} \quad \dots (1)$$

Where,  $\lambda$  the wavelength of X-ray used ( $\lambda = 1.54090 \text{ \AA}$ ),  $\beta$  is full width at half maxima and  $\theta$  is diffraction angle. The lattice parameters were estimated as  $a = 3.104$ ,  $b = 7.513$ ,  $c = 4.766$  and unit cell volume 111.02. The dislocation density ( $\delta$ ), the number of crystallites per unit area (N) and the strain ( $\epsilon$ ) of the films were determined by following relations:

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

$$N = t / D^3 \quad \dots (3)$$

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

Where, t is the thickness of the film. The calculated structural parameters are  $\delta = 2.047 \times 10^{14} \text{ lines / m}^2$ ,  $N = 9.264 \times 10^{17}$ ,  $\epsilon = 0.9926$ . The small values of  $\delta$  obtained in the present study confirm the good crystallinity of the thin films fabricated by the closed space sublimation.

#### 3.2. Morphological Analysis

The surface morphology of (CdS)<sub>0.6</sub>Te<sub>0.4</sub> thin film were analyzed by Scanning Electron Microscope. Figure 2 shows the micrograph of (CdS)<sub>0.6</sub>Te<sub>0.4</sub> thin film.

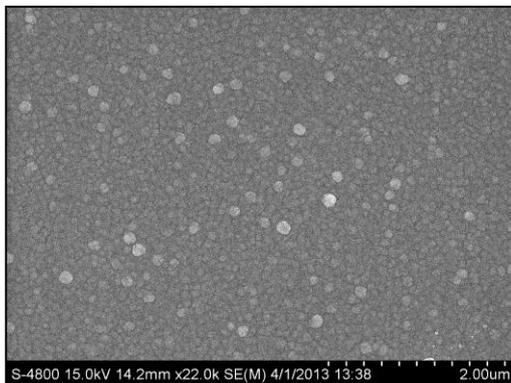


Fig.2. SEM Micrograph of (CdS)<sub>0.6</sub>Te<sub>0.4</sub> Thin Film

From SEM image it is observed that as deposited (CdS)<sub>0.6</sub>Te<sub>0.4</sub> thin film is uniform with dense surface morphology covering entire surface area of substrate without any defects like crack and pinhole. The grain size is found to be within the range of 74-170 nm. This may be due to multiple grain fusion together and form cluster type formation.

### 3.3. EDAX Analysis

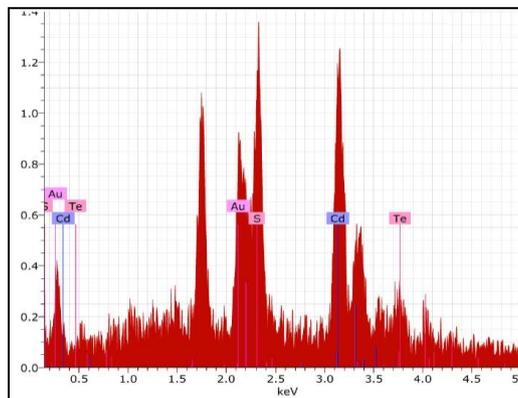


Fig.3. EDAX Spectrum of (CdS)<sub>0.6</sub>Te<sub>0.4</sub> Thin Film

The quantitative analysis of the sample was carried out by using EDAX technique attached with the SEM assembly. Figure 3 shows EDAX spectrum of (CdS)<sub>0.6</sub>Te<sub>0.4</sub> thin film. The elemental analysis was carried out for Cadmium, Sulfur and Telluride. The average atomic percentage was found as 47.31: 47.01: 5.67. The Au is present due to the gold coating at the time of SEM characterization.

### 3.4. Optical Analysis

Optical analysis of the samples was carried out by recording absorbance and transmittance spectra in the wavelength range of 300 – 900 nm. Figure 4 shows the absorbance spectra while transmittance of the (CdS)<sub>0.6</sub>Te<sub>0.4</sub> thin films is shown in inset.

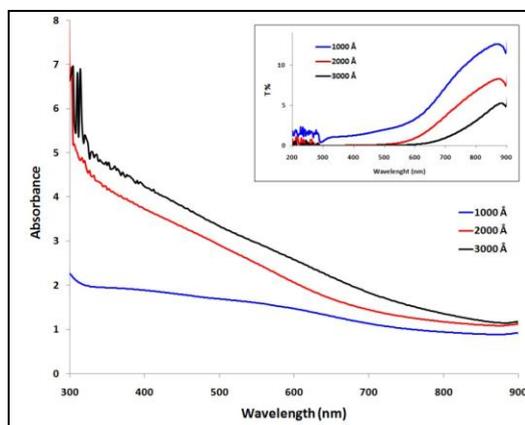


Fig.4. Plot of wavelength Vs. Absorbance

The films have transmittance below the 14% because of blackish color of Telluride. Figure 4 reveals that as the thickness of the film increases; the absorbance gets increases while transmittance gets decreases. The optical band gap of these films has been calculated using the Tauc relation:

$$\alpha h\nu = A (h\nu - E_g)^n \quad \dots (5)$$

Where,  $h\nu$  is the photon energy,  $\alpha$  is the absorption coefficient,  $E_g$  is the band gap and  $A$  is constant. The optical band gap was find out from the plot of  $(\alpha h\nu)^2$  Vs.  $E_g$  as shown in figure 5.

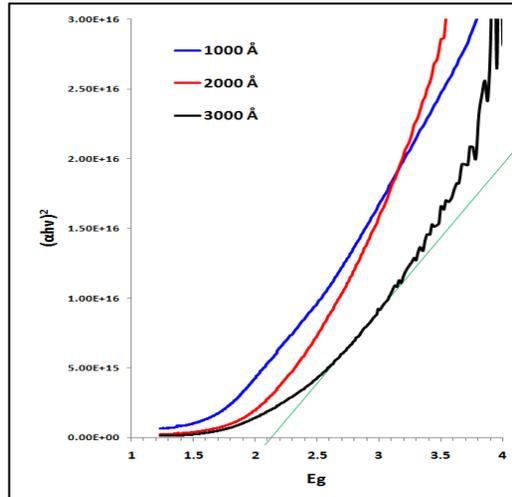


Fig.5. Plot of Optical Band Gap

The straight line portion is extrapolated to cut the x-axis, which gives the optical energy band gap. All graphs show straight line portions supporting the interpretation of direct band gap for all the films. The optical band gap of (CdS)<sub>0.6</sub>Te<sub>0.4</sub> thin films has been found to be within the range of 1.6 to 2.1 eV.

### 3.5. Electrical Analysis

The four probe method was carried out to find out the electrical resistivity and activation energy of the (CdS)<sub>0.6</sub>Te<sub>0.4</sub> thin films. Figure 6 shows the plot of I-V characteristics at room temperature while figure 7 represents the plot of log ρ Vs (1000/T) for various thicknesses, shows that resistivity variation follows the relation:

$$\rho = \rho_0 \exp \left( \frac{E_a}{kT} \right) \quad \dots (6)$$

Where, k is Boltzmann constant, T is temperature and E<sub>a</sub> is activation energy.

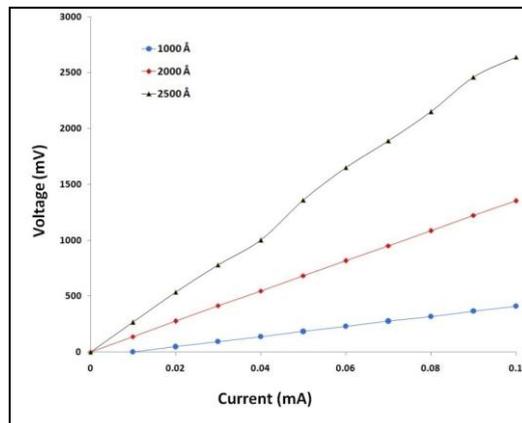


Fig.6. Plot of I-V Characteristics

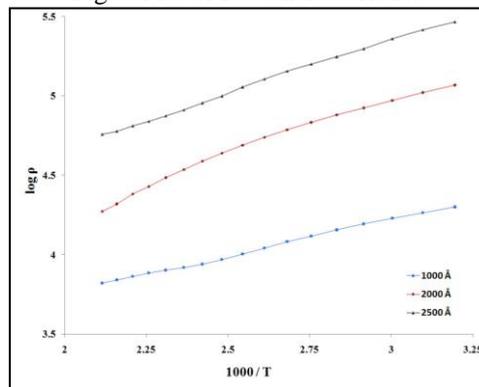


Fig.7. Plot of Log ρ Vs. 1000/T

The resistivity of semiconductor is depends upon the carrier concentration, temperature and mobility. The carrier concentration is positive function of temperature due to the thermal excitation of electrons. The conductivity increases, as the Fermi energy moves further into the energy gap way from the conduction band toward valance band. The electrical resistivity and activation energy with the various thicknesses of (CdS)<sub>0.6</sub>Te<sub>0.4</sub> thin film is mentioned in the Table 1.

**Table 1 Electrical Resistivity and Activation Energy**

Thickness (Å)	Electrical Resistivity (Ω-cm)	Activation Energy (eV)
1000	0.2045	0.01822
2000	1.2285	0.02899
2500	3.0811	0.02697

### 3.6. Thermo Electric Power Analysis

The thermo electric power is defined as the ration of thermo electric voltage to the change in temperature across a piece of semiconductor, using the relation:

$$S = -\Delta V / \Delta T \quad \dots (7)$$

The conduction is done from hot to cold end in n-type. Figure 8 shows the graphical relations of seebeck coefficient and temperature difference whereas the relationship of thermo emf and change in temperature is shown in inset. The thermo emf and seebeck coefficient are observed as a function of temperature. The Fermi energy was estimated by:

$$E_F = eST - AKT \quad \dots (8)$$

Where, e is electronics charge, S is seebeck coefficient, K is Boltzmann constant and T is absolute temperature.

**Table 2 Fermi Energy and Scattering Coefficient**

Thickness (Å)	Fermi energy (eV)	Scattering Coefficient
1000	0.2628	2.3188
1500	0.1002	2.2840
3000	0.4528	2.4347

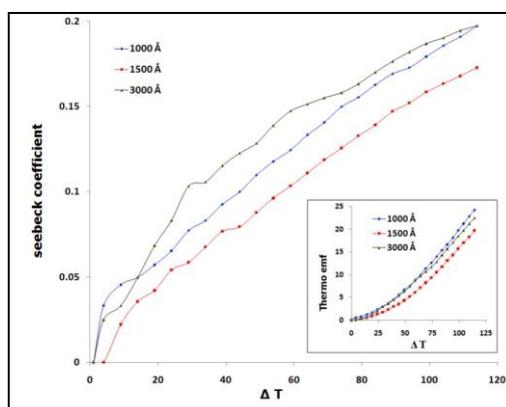


Fig.8. Plot of Seebeck Coefficient Vs. Δ Temperature

## IV. Conclusion

The XRD confirms the polycrystalline nature with monoclinic crystal structure of the deposited thin films. Scanning electron microscopy studies revealed uniform deposition having average grain size of 74-170 nm. The elemental analysis was carried out by EDAX for Cd, S and Te. The optical band gap was found to be 1.6 – 2.1 eV. The thermo electric power measurements revealed that films exhibit n-type of conductivity. Electrical analysis illustrates that the (CdS)<sub>0.6</sub>Te<sub>0.4</sub> films can be used in optoelectronic devices.

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