

## Characterization of Hot Wall Deposited CdSe<sub>0.6</sub>Te<sub>0.4</sub> Thin Films

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**Abstract:** CdSe<sub>x</sub>Te<sub>1-x</sub> thin films are of great practical interest owing to their unique properties, which make them suitable for solar cell applications. By varying the Se and Te contents, the band gap can be suitably tailored to fit for selected applications. In our present work we have deposited CdSe<sub>0.6</sub>Te<sub>0.4</sub> thin films onto glass substrates by hot wall deposition technique using the synthesized CdSe<sub>0.6</sub>Te<sub>0.4</sub> compound. CdSe<sub>0.6</sub>Te<sub>0.4</sub> compound has been synthesized by direct reaction of elemental cadmium, selenium and tellurium taken in suitable weight proportion. The hot wall setup consists of quartz tube over which kanthal wire is wound with equal spacing to get uniform heat distribution through out the tube. The X-ray diffraction studies were carried out on all the deposited CdSe<sub>0.6</sub>Te<sub>0.4</sub> films and it revealed that the films are polycrystalline in nature exhibiting both hexagonal and cubic phases. The composition of the films has been studied using energy dispersive X-ray analysis (Cd = 49.10 at%, Se = 29.05 at % and Te = 21.85 at %). The optical properties of the films have been studied using the UV-Vis-NIR spectrophotometer and from the transmittance spectra the optical parameters like band gap, refractive index and absorption coefficient has been evaluated. The CdSe<sub>0.6</sub>Te<sub>0.4</sub> films were found to have direct band gap. The band gap and refractive index have been found to be 1.48 eV and 2.2 respectively.

**Keywords:** Hot wall deposition, CdSe<sub>0.6</sub>Te<sub>0.4</sub> thin films, structure, optical properties

### 1. INTRODUCTION

Thin films of cadmium chalcogenides have become promising materials for applications in electro - optic devices and photo electrochemical solar cells. Presently, one of the best material where tailoring of band gap is possible is from the group of cadmium chalcogenides [1,2], viz., n-CdSe<sub>0.6</sub>Te<sub>0.4</sub> which has a band gap very close to the maximum absorption in the visible spectrum  $\approx$  1.45 eV [3]. Power conversion efficiency up to 8% has been obtained using polycrystalline thin films of CdSe<sub>0.65</sub>Te<sub>0.35</sub> which has an optical band gap similar to that of CdTe and shows stability comparable to CdSe in sulphide – polysulphide electrolyte [4]. CdSe<sub>x</sub>Te<sub>1-x</sub> thin films have been prepared by several workers by different methods such as thermal evaporation of pre-reacted samples in vacuum [5,6], co-evaporation of CdSe and CdTe powders [7], electron beam evaporation [8], flash evaporation [9], chemical methods [10] and hot wall deposition [11-13]. The thermal evapo-

ration or related techniques in vacuum lead to the evaporation of the compound at different vapor pressures owing to the differences in the evaporation temperatures of the constituent elements, which result in non- stoichiometric films.

In the present work we report about the hot wall deposition process, which is used to prepare CdSe<sub>0.6</sub>Te<sub>0.4</sub> thin films along with the structural and optical properties of the deposited films. Hot wall deposition technique is the method by which epitaxial films of congruently evaporating compound semiconductors can be prepared with bulk like properties [14]. Schikora et al [15] have claimed that CdTe films deposited on GaAs substrates by hot wall deposition technique show superior luminescence properties when compared to molecular beam epitaxy (MBE) and metal organic chemical vapor (MOCVD) deposited films.

### 2. EXPERIMENTAL TECHNIQUES

CdSe<sub>0.6</sub>Te<sub>0.4</sub> compound has been prepared by direct reaction of high purity elemental cadmium, selenium and tellurium. Stoichiometric amounts of cadmium, selenium and tellurium are

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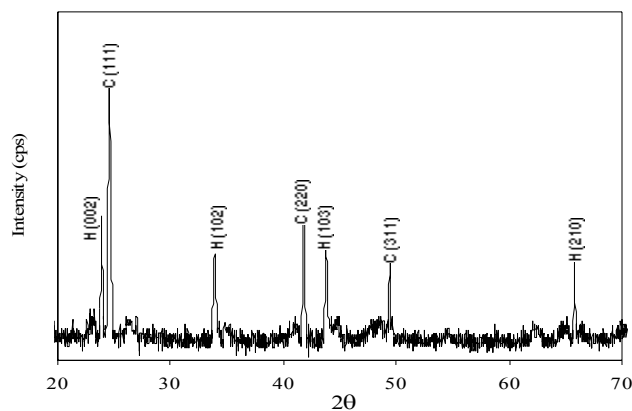


Figure 1. X-ray diffractogram of bulk  $\text{CdSe}_{0.6}\text{Te}_{0.4}$

taken in a quartz tube and the pressure in the ampoule (quartz tube) is reduced to  $10^{-4}$  Torr. The quartz ampoule is gradually heated at a rate of 100 K/hr in steps up to 1200 K. The ampoule is maintained at this temperature for about 4 hours and then cooled slowly to room temperature. During the process of heating and cooling the ampoule is rotated continuously to ensure homogeneity in the molten mixture.  $\text{CdSe}_{0.6}\text{Te}_{0.4}$  thin films have been deposited on to well-cleaned glass substrates by hot wall deposition technique. Hot wall deposition technique is the method by which films can be deposited under conditions very close to thermodynamic equilibrium with minimum loss of material. The main feature of the hot wall system is the heated linear quartz tube, which serves to enclose and direct the vapor from source to substrate. The hot wall system used in the present study consists of a quartz tube of length 6.5 cm and diameter 1 cm with one end open and the other end closed. The source material is taken in the quartz tube. On the top of the tube the substrate was held at a distance of less than 1 mm, which acts almost as a lid closing the tube. Kanthal wire wound along the length of the quartz tube serves as wall heater. The quartz tube and the heater coils are placed inside the vacuum chamber in which a pressure of  $10^{-5}$  Torr is achieved.  $\text{CdSe}_{0.6}\text{Te}_{0.4}$  thin films have been deposited with wall temperature around 700 K. Due to radiation from the hot wall the substrate temperature automatically raised to 340K during deposition. In our preliminary work we have already optimized the heat distribution inside the tube. The structure of the deposited films has been studied using X-ray diffractometer (model JEOL 8030 Japan) fitted with monochromatic  $\text{Cu-K}\alpha$  radiation. Thickness of the deposited films has been measured using multiple beam interferometric technique. The composition of the deposited films has been determined by energy dispersive X ray analysis (Leica S 440i). The transmittance spectra of the deposited films have been recorded using JASCO UV-VIS-NIR spectrophotometer (model V 570).

### 3. RESULTS AND DISCUSSION

The X-ray diffraction pattern of  $\text{CdSe}_{0.6}\text{Te}_{0.4}$  compound and thin film is shown in figures 1 and 2 respectively. The presence of sharp peak confirms the polycrystalline nature of the material.  $\text{CdSe}_{0.6}\text{Te}_{0.4}$  compound and thin films are found to have both the

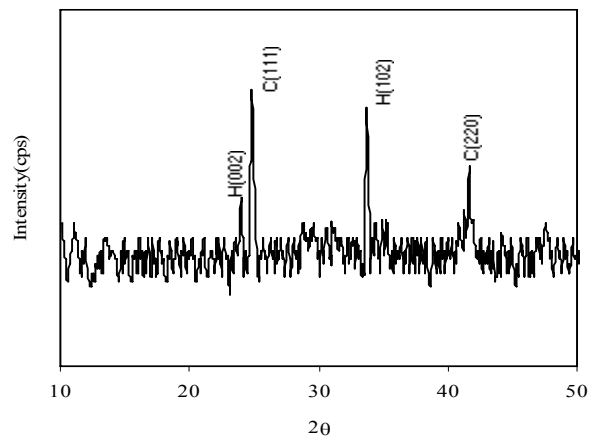


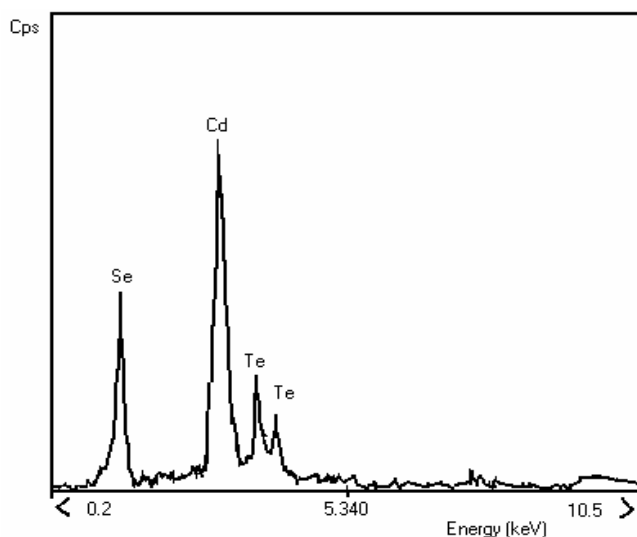
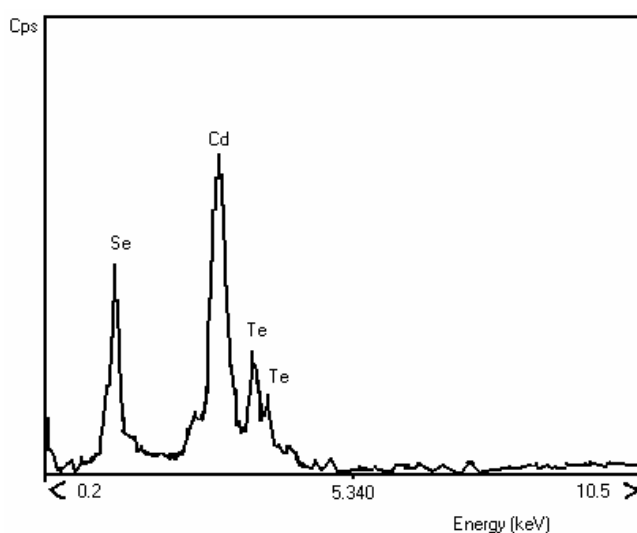
Figure 2. X-ray diffractogram of  $\text{CdSe}_{0.6}\text{Te}_{0.4}$  thin film of thickness 1110 Å

Table 1. Microstructural parameters of  $\text{CdSe}_{0.6}\text{Te}_{0.4}$  thin film

Structure	Grain size (Å)	Dislocation Density (lines/m <sup>2</sup> )	Strain
Cubic	515	$3.760 \times 10^{14}$	$8.351 \times 10^{-4}$
Hexagonal	598	$3.454 \times 10^{14}$	$5.344 \times 10^{-4}$

cubic zinc blende and hexagonal wurtzite phase. A mixture of separate phases of both CdSe and CdTe is observed. Similar observations of the presence of both the cubic zinc blende and hexagonal wurtzite phase for  $\text{CdSe}_{0.6}\text{Te}_{0.4}$  has been reported by earlier workers [16-19]. They have reported that for  $0 \leq x \leq 0.4$ , this system exhibits the cubic structure and for  $0.7 < x < 1$  it has the hexagonal symmetry. For the composition  $x \approx 0.6$  the cubic and hexagonal phases were found to coexist in the system. The grains are found to have a preferred orientation along the (111) and (102) directions corresponding to the cubic and hexagonal phases respectively. The lattice parameter values have been calculated for the prepared bulk and are  $a = 6.260$  Å for the cubic phase and  $a = 4.322$  Å,  $c = 7.437$  Å for the hexagonal phase. For thin film of thickness 1110 Å the lattice parameter values were  $a = 6.190$  Å for the cubic phase and  $a = 4.393$  Å,  $c = 7.406$  Å for the hexagonal phase. The lattice parameter values of the thin film are found to be nearly the same as that of the bulk. The  $c/a$  ratio for the wurtzite phase of the prepared  $\text{CdSe}_{0.6}\text{Te}_{0.4}$  bulk and thin film are 1.720 and 1.685 respectively. The theoretical value of  $c/a$  ratio for wurtzite structure is 1.633. The zinc blende and wurtzite structures have the same primary coordination, with each cation surrounded by four nearest neighbor anions in tetrahedral configuration and vice versa. This close structural relationship, together with the chemical similarity between tellurium and selenium, explains the broad range of mutual solid solubility exhibited by CdTe and CdSe [20]. The grain size of the deposited films has been determined using Scherer's formula. The microstructural parameters such as grain size, strain and dislocation density have been calculated and are as given in Table 1. The grain size of the hexagonal phase is found to be larger than the cubic phase.

The chemical constituents present in the bulk and thin film of  $\text{CdSe}_{0.6}\text{Te}_{0.4}$  has been determined using energy dispersive X-ray analysis. The EDAX pattern of  $\text{CdSe}_{0.6}\text{Te}_{0.4}$  bulk and the thin film are shown in figures 3 and 4 respectively. The bulk and thin film

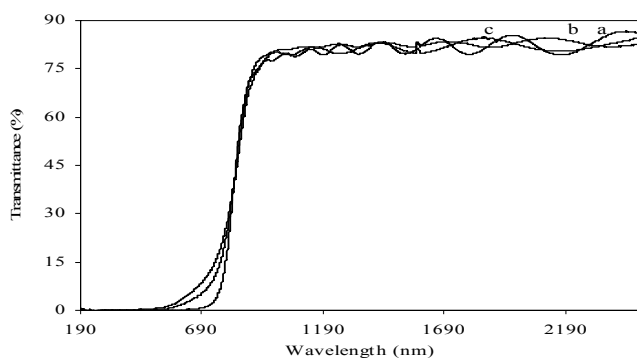
Figure 3. EDAX pattern of bulk CdSe<sub>0.6</sub>Te<sub>0.4</sub>Figure 4. EDAX pattern of CdSe<sub>0.6</sub>Te<sub>0.4</sub> thin film of thickness 1110 Å

are found to exhibit a composition of Cd – 50.65 at%, Se – 28.95 at%, Te – 20.40 at% and Cd - 49.10 at%, Se – 29.05 at% , Te – 21.85 at% respectively. The EDAX results show that the prepared CdSe<sub>0.6</sub>Te<sub>0.4</sub> thin film and bulk have almost the same composition. Generally II-VI compounds undergo complete dissociation during evaporation and the films are grown by allowing the constituent vapors to react with each other at the substrate at elevated temperatures. But by hot wall deposition technique the dissociation can be avoided by suitably adjusting the wall and source temperatures. This indicates that excellent composition control can be easily achieved by hot wall deposition technique.

Fig. 5 shows the transmittance spectra of CdSe<sub>0.6</sub>Te<sub>0.4</sub> thin films of different thicknesses deposited by hot wall deposited technique. The films show good transparency exhibiting interference pattern in the wavelength region 900 nm to 2500 nm. In the region of the spectrum where the thin film is transparent, the transmission spectrum exhibits oscillatory behavior due to interference between the wave fronts reflected from the two surfaces of the thin films [21]. The value of absorption coefficient ( $\alpha$ ) was calculated for all the films. The study of the absorption coefficient in the fundamental region and near the fundamental edge provides valuable information about inter band transitions and consequently about the energy band structure of the material. The electronic transition between the valence and conduction bands can be direct or indirect. In both cases it can be allowed as permitted by the transition probability ( $p$ ) or forbidden where no such probability exists. The transition probability is given by the equation

$$(\alpha h\nu)^p = A (h\nu - E_g)$$

where  $E_g$  denotes the band gap,  $h\nu$  the energy of the incident photon and  $A$  is a constant. The exponent  $p$  is the number which characterizes the transition process,  $p = 2$  for direct allowed transitions,  $p = 2/3$  for direct forbidden transitions,  $p = 1/2$  for indirect allowed transitions and  $p = 1/3$  for indirect forbidden transitions. The band gap  $E_g$  is determined by plotting  $(\alpha h\nu)^p$  against photon energy  $h\nu$  for suitable value of  $p$  the graph is a straight line

Figure 5. Transmittance spectra of CdSe<sub>0.6</sub>Te<sub>0.4</sub> thin films of different thicknesses (a = 1110 Å, b = 1545 Å, c = 2110 Å)

and the value of band gap ( $E_g$ ) is obtained by extrapolating the linear portion of the curve to intercept the photon energy axis.

The plots  $(\alpha h\nu)^{2/3}$  versus  $h\nu$  direct forbidden,  $(\alpha h\nu)^{1/2}$  versus  $h\nu$  indirect allowed,  $(\alpha h\nu)^{1/3}$  versus  $h\nu$  indirect forbidden of CdSe<sub>0.6</sub>Te<sub>0.4</sub> thin films of different thicknesses did not exhibit a straight-line behavior over any part of the optical spectrum. The absence of straight-line behavior in these plots (not shown) reveals that the type of transition in CdSe<sub>0.6</sub>Te<sub>0.4</sub> thin films is neither direct forbidden nor indirect. Plot of  $(\alpha h\nu)^2$  versus  $h\nu$  of CdSe<sub>0.6</sub>Te<sub>0.4</sub> thin films of different thicknesses are shown in Fig. 6. The straight-line nature of the plot reveals that the nature of transition in hot wall deposited CdSe<sub>0.6</sub>Te<sub>0.4</sub> thin films is direct allowed. Intercept of the linear portion of the plot on the  $h\nu$  axis of Fig. 6 gives the value of direct band gap of the films. The band gap has been found to be 1.49, 1.48 and 1.48 eV for films of thicknesses 1110 Å, 1545 Å and 2110 Å. Bouroushian et al [22] and Islam et al [23] have reported almost the same band gap for CdSe<sub>0.6</sub>Te<sub>0.4</sub> thin films deposited by cathodic electro deposition and electron beam evaporation respec-

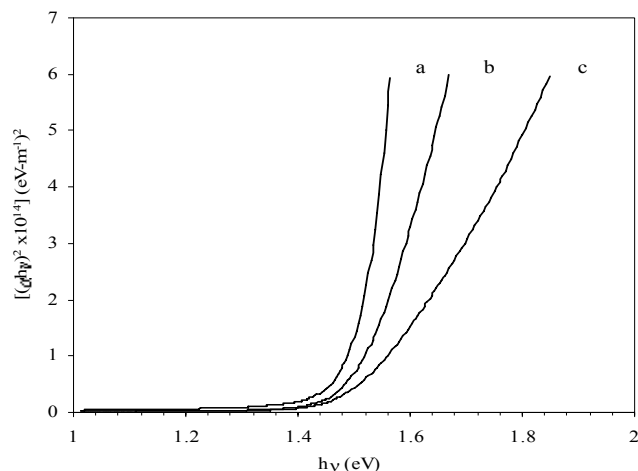


Figure 6. Plot of  $(\alpha hv)^2$  versus  $h\nu$  of  $\text{CdSe}_{0.6}\text{Te}_{0.4}$  thin films of different thicknesses (a = 1110 Å, b = 1545 Å, c = 2110 Å)

tively. A similar band gap value has been reported by several other earlier workers [3,24-27]. It is observed that there is no appreciable change in the band gap with film thickness. Hence it is possible to obtain thin films of Cd (Se, Te) with the required optimum band gap ( $1.4 \pm 0.1\text{eV}$ ) for solar cell applications using this simple hot wall deposition technique.

Refractive indices of the films were calculated from the transmission curves using the interference fringe region of the transmittance spectrum by the method of Manifacier et al [28]. In this method the maximum transmittance ( $T_{\max}$ ) and minimum transmittance ( $T_{\min}$ ) were considered to be continuous function of wavelength through refractive index  $n(\lambda)$  and absorption coefficient ( $\alpha$ ). From these functions which are the envelopes of the maxima  $T_{\max}(\lambda)$  and minima  $T_{\min}(\lambda)$  of the transmittance curves, the refractive indices of the films are calculated using the relations by Manifacier et al.

$$n^2 = N + (N^2 - n_0^2 n_1^2)^{1/2}$$

$$N = (n_0^2 + n_1^2) / 2 + 2n_0 n_1 (T_{\max} - T_{\min}) / (T_{\max} \times T_{\min})$$

where  $n_0$  and  $n_1$  are the refractive indices of air and glass respectively. The variation of the refractive index ( $n$ ) with wavelength ( $\lambda$ ) of  $\text{CdSe}_{0.6}\text{Te}_{0.4}$  films of different thicknesses is shown in figure 7. The refractive index of the deposited  $\text{CdSe}_{0.6}\text{Te}_{0.4}$  thin films is found to show no appreciable variation with the increase of incident photon wavelength in the wavelength region 1000nm to 2500nm. The observed value of refractive index, which is in the range 2.21 to 2.37, is slightly less than the value of 2.6 to 2.9 reported by earlier workers [8,29].

#### 4. CONCLUSION

$\text{CdSe}_{0.6}\text{Te}_{0.4}$  films have been deposited by hot wall deposition technique using the synthesized compound. In the  $\text{CdSe}_{0.6}\text{Te}_{0.4}$  bulk and thin films it has been observed that both the cubic and hexagonal phases coexist. The band gap and refractive index of the films have been calculated and are found to show no appreciable variation with film thickness.

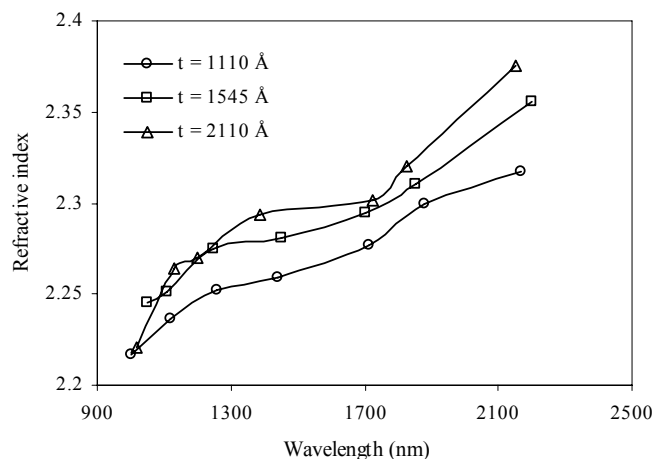


Figure 7. Variation of refractive index with wavelength of  $\text{CdSe}_{0.6}\text{Te}_{0.4}$  thin films

#### 5. ACKNOWLEDGEMENT

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