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# Optical properties of vacuum evaporated $Cd_xSn_{1-x}Se$ polycrystalline thin films: influence of composition and thickness

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**Abstract**

Polycrystalline $Cd_xSn_{1-x}Se$ material is synthesized by melt growth technique for various $x$ values and thin films are prepared by vacuum evaporation technique. Optical transmittance measurements have been made on thin films of $Cd_xSn_{1-x}Se$, with $x = 0, 0.3, 0.75$ and 1 for various thicknesses. The studies reveal that these thin films have a direct allowed band gap energy and the indirect band gap energy is improbable. The band gap energy increases with decrease in thickness in all the compositions and it is attributed to the quantum size effect.


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*Keywords:* Transmittance; Optical band gap; Vacuum deposition; Quantum size effect

## 1. Introduction

Metal selenide thin films offer a range of optical band gap energies suitable for various optical and optoelectronic applications. Thin films of tin selenide have great potential applications, such as memory switching devices [1]. CdSe thin films have found applications in solar cells, thin film transistors [2,3] and gamma-ray detectors [4]. CdSe and SnSe have been studied in the form of both thin films and single crystals [5–8]. CdSe is a narrow band semiconductor and its optical band gap is 1.74 eV [9], whereas SnSe have the band gap energy of 0.9 eV [10]. This difference in energy gap lies in the optical absorption spectrum of solar radiation and hence the study of the optical properties of $Cd_xSn_{1-x}Se$ with $x = 0, 0.3, 0.75$ and 1 thin films is carried out. No study has been

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reported in the literature for $Cd_xSn_{1-x}Se$ solid solutions either in the form of thin films or single crystals. This paper characterizes the band gap energy and optical absorption coefficient of SnSe, $Cd_{0.3}Sn_{0.7}Se$, $Cd_{0.75}Sn_{0.25}Se$ and CdSe thin films prepared by vacuum deposition technique.

## 2. Experimental methods

The bulk $Cd_xSn_{1-x}Se$ materials with $x = 0, 0.3$ and 0.75 were synthesized in a quartz ampoule by mixing cadmium metal, tin and selenium (Aldrich, 99.99% pure) powders in their stoichiometric ratio by melt growth technique. The synthesized compound was analyzed by X-ray diffraction technique for their homogeneity and crystalline nature. The composition analysis of the synthesized powder materials was carried out using atomic absorption spectrophotometer.

The synthesized $Cd_xSn_{1-x}Se$ materials with $x = 0, 0.3$ and 0.75 and commercially available CdSe powder sample (Aldrich, 99.99% pure) were used to deposit thin films using Hind Hivac Vacuum Coating unit (model-12-A4) at different substrate temperatures and thicknesses. The powder materials were kept in a molybdenum boat during evaporation and the resistive evaporation technique was used to prepare thin films. The X-ray powder diffraction patterns for the synthesized $Cd_xSn_{1-x}Se$ with $x = 0, 0.3$ and 0.75 powder materials and CdSe powder material and thin films were recorded in JEOL JDX 8030 X-ray diffractometer using Cu Kα radiation at room temperature. The X-ray photoelectron spectroscopy (XPS) spectra were recorded for $Cd_xSn_{1-x}Se$ thin films in an ESCALAB MK II spectrometer (VG Scientific Ltd., UK) using Mg Kα radiation of energy 1253.6 eV. The optical transmission spectrum was recorded using a HITACHI model V-3400 UV-Vis-NIR spectrophotometer in the region 400–2000 nm. All the measurements were carried out at room temperature for normal incidence mode. The transmittance of the thin films was measured relative to that of an identical uncoated substrate. The estimated measurement error including the instrumental error in transmittance is less than 1%. Thin film uniformity was checked by measuring the transmission curves at different areas of the film.

## 3. Results and discussion

### 3.1. Structure and composition

The X-ray powder diffraction data recorded for $Cd_xSn_{1-x}Se$ powder materials with $x = 0, 0.3, 0.75$ and 1 reveal that these powder materials are polycrystalline in nature. The XRD peaks are indexed with the help of the software DICVOL91 [11,12] and Hull and Davey chart [13]. The lattice parameters are evaluated using the indexed *hkl* values and the measured $2\theta$ values using the software UNITCELL [14]. The refined cell parameters for all the materials are given in Table 1. CdSe powder material shows that it crystallizes in hexagonal crystal system, whereas SnSe, $Cd_{0.3}Sn_{0.7}Se$ and $Cd_{0.75}Sn_{0.25}Se$ powder materials show that they crystallize in orthorhombic crystal system as reported [15].

The XRD patterns recorded for the $Cd_xSn_{1-x}Se$ thin films with $x = 0, 0.3, 0.75$ and 1 are found to be polycrystalline in nature and their crystallinity increases with annealing. The XRD data recorded agrees well with the standard one. The composition of $Cd_xSn_{1-x}Se$ thin films with $x = 0.3, 0.75$ and 1 is found to be rich in selenium (1–3%) and cadmium deficient and is displayed in Table 2. The SnSe thin film is found to be selenium deficient.

### 3.2. Optical band gap energy

The optical absorption coefficient α is determined using the relation:

$$\alpha = \frac{2.303}{t}\log_{10}\left(\frac{1}{T}\right), \tag{1}$$

where $t$ is the thickness of the film and $T$ is the transmittance. The relation [16] between the photon energy and the optical absorption coefficient is

$$\alpha h\nu = A(h\nu - E_g \pm E_p)^x, \tag{2}$$

where $E_g$ is the energy gap, $E_p$ is the energy of the absorbed (+) or emitted (−) phonon energy. For