Synthesis and Characterization of Nanostructured Thin Films of (CdS)_{0.6} Se_{0.4} for Solar Cell

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Abstract: The high quality thin films of $(CdS)_{0.6}$ Se_{0.4} have been synthesized using thermal evaporation technique onto precleaned rotating amorphous glass substrate at room temperature. The films were characterized by X-Ray Diffractometer, Scanning Electron Microscopy, Atomic Force Microscopy and UV-VIS Spectrophotometer. The XRD spectrum illustrates that the films are polycrystalline having hexagonal structure. AFM images reveals that, sample is smooth with well defined nano sized grains. SEM shows that all the grains are spherical in nature and grains forming conglomerate to form a cluster. The optical band gap energy was estimated within 1.95 to 2.05 eV by using UV-VIS Spectrophotometer. Keywords:XRD, SEM, AFM and UV-VIS

I. Introduction

From several years, nanocrystalline semiconductor thin films have received much attention, because of their properties such as energy band structure. The band gap of the semiconductor materials can be significantly modify with the help of doping [1].

The II-VI group semiconductors are important materials due to their commercial use in various applications in optoelectronic devices [2] in fabrication of thin film transistor [3], solar cells [4, 5], gas sensors [6], and lightemitting diodes [7]

The nanocrystalline thin films of II–VI semiconductor has been a rapidly developing area of research. The thin film synthesis technique alters the properties of the films. There are various techniques for the synthesis of thin films, sputtering [8], thermal Evaporation [9,10], MBE [11], CBD [12,13], spray pyrolysis [14] electron beam deposition [15].

The vacuum evaporation is a very reliable technique for synthesis of thin film. The thin films prepared by vacuum evaporation technique are uniformed with excellent crystallinity, dense and highly oriented. The qualities and properties of film mainly depend upon pressure, deposition rate, substrate temperature and thickness of the film [16].

In the present paper investigation structural / morphological and optical properties of CdS-Se thin films were carried out.

2.1. Preparation of Alloy

II. Research Elaborations

The $(CdS)_{0.6}$ Se_{0.4} compound ingots were obtained by taking appropriate amount of 99.999% pure CdS and Se in an evacuated quartz ampoule. The ampoule with the charge was then sealed under a pressure of 10⁻⁶ mbar and was placed in rotating furnace. The temperature of the furnace was raised gradually to 900°C and left at this temperature for about 12 hrs. Well mixed charges were then quenched in an ice bath. The (CdS)_{0.6} Se_{0.4} ingot was taken out from the ampoule and used for film preparation.

2.2. Synthesis of Thin Films

The ternary alloy of Cadmium Sulphoselenium $(CdS)_{0.6}Se_{0.4}$ thin films have been deposited on rotating glass substrate, by thermal evaporation technique under vacuum of 10^{-5} torr. The substrate to source distance was kept at 14 cm. The samples with various thicknesses were deposited under similar conditions. The thickness of the films was monitored by quartz crystal thickness monitor (DTM-101) provided by Hind-Hi Vac. The deposition rate was maintained 10-12 Å/sec throughout sample preparation. Before evaporation, the glass substrates were cleaned throughout using concentrated chromic acid, detergent, acetone and distilled water.

2.3. Characterization Techniques

X - Ray diffractograms (Bruker, Germany - CuK α line) were obtained of these samples to study crystallinality and structural information. The scanning angle (2 θ) was within the range of 20° - 80°. The morphology and microstructure of the samples were characterized by Scanning Electron Microscope (Zeiss - EVO 50), operating with an accelerating voltage 10 KV and Atomic Force Microscopy (AFM). The elemental

analysis of the sample was carried out by EDAX (Energy dispersive X-ray Analyzer) technique attached with SEM. Optical band gap was measured with the help of UV-VISSpectrophotometer (Shimadzu – 2600).

III. Results

3.1. X-Ray Diffractometer (XRD)

Figure 1 shows the XRD pattern of $(CdS)_{0.6}Se_{0.4}$ thin films of thickness 3000Å. The 2 θ peaks observed at 25.0°, 26.5° which correspond to the (100), (002) planes of reflections.



Fig.1. XRD Spectrum of CdS_{0.6}Se_{0.4} Thin Film with Thickness 3000Å

The presence of large number of peaks indicates that the films are polycrystalline in nature having hexagonal in shape. The strong and sharp diffraction peaks show the formation of well crystalline sample. The intensity of the peaks depends on crystalline quality. The average grain size is found to be 178.6 nm by Debye - Scherrer formula:

$$d = \frac{0.9\lambda}{\beta\cos\theta} \qquad \dots \dots (1)$$

where, λ the wavelength of X-ray used ($\lambda = 1.64060$ Å), β is full width at half maxima and θ is diffraction angle. The lattice parameters was found to be a = 4.154 and b = 6.764Å. The unit cell volume was estimated as 101.08Å³

3.2. Atomic Force Microscopy (AFM)

The surface morphology of $(CdS)_{0.6}Se_{0.4}$ thin film was investigated by Atomic Force Microscopy. Figure 2 shows 3D AFM images, having 100 µm × 100 µm areas of the deposited films.



Fig.2. AFM of (CdS)_{0.6}Se_{0.4} Thin Film with Thickness 3000Å

The AFM images reveal that, the sample is smooth and well covered almost area of substrate. The particles are found to be arranged almost in a uniform size distribution. Some particles are found to be elongated niddle shape because of overlapping.

3.3. Scanning Electron Microscopy (SEM)

Figure 3 shows SEM micro photograph of $CdS_{0.6}Se_{0.4}$ thin film of thickness 3000Å.



Fig.3. SEM of (CdS)_{0.6}Se_{0.4} Thin Film with Thickness 3000Å

The SEM image of $(CdS)_{0.6}Se_{0.4}$ thin film illustrates that the film is homogeneous and grains are uniformly distributed, well cover substrate area and free from defect like fracture or peeling. These uniformly distributed nano-sized grains over smooth homogeneous background forms clusters with various sizes ranging from 167-238 nm.

3.4. EDAX:

The elemental analysis was carried out for detecting the atomic percentage of element presented on the film. Figure 4 shows EDAX pattern of the $(CdS)_{0.6}Se_{0.4}$ thin film.



Fig.4. EDAX Spectrum of (CdS)_{0.6}Se_{0.4} Thin Film with Thickness 3000Å

The elemental analysis was carried out by EDAX method. The presences of Cd, S and Se with their atomic percentage 44.98: 34.14: 20.88 was found respectively. Recorded EDAX spectrum revels that there is no evidence of other impurity. It indicates that purity of deposited film.

3.5. UV-VIS Spectroscopy:

The optical assets like absorbance, transmittance and optical band gap were determined by employing a Shimadzu 2460 UV-VIS Spectrophotometer within the range of 200 - 900nm wavelength range. Figure 5 and 6 shows the absorbance and transmittance spectra respectively.



Fig.5. Absorbance Spectrum of (CdS)_{0.6}Se_{0.4} Thin Films



Fig.6. Transmittance Spectrum of (CdS)_{0.6}Se_{0.4} Thin Films

Figure 5 and 6 revels 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 estimated from the absorbance spectrum. Figure 7 clearly shows the linear dependence of Eg upon the thickness.



Fig. 6 Plot of Optical Band Gap of (CdS)_{0.6}Se_{0.4}Thin Films

The linear portion is extrapolated to cut the x-axis, which gives the energy gap. The $(CdS)_{0.6}Se_{0.4}$ layer has the transmittance lower than 100 % at wavelengths longer than the absorption edge. The estimated band gap varies between 1.95 to 2.05eV. Hence the $(CdS)_{0.6}Se_{0.4}$ can be used in fabrication of solar cell application.

IV. Conclusions

The thin films of $(CdS)_{0.6}Se_{0.4}$ were deposited on rotating glass substrate by thermal evaporation techniques. The XRD study illustrates that the films are polycrystalline in nature having hexagonal structure. The AFM images reveals that, sample consists of well defined nano sized grains with almost uniform size distribution. SEM reveals that films were uniformly deposited over the substrate and particles were found to be spherical in shape. The incorporation of Cd, S and Se was confirmed through EDAX spectrum. Optical band gap was found to be 1.95 to 2.05eV. The band gap is found to be a function of thickness which can be used for efficient photo cells and photo voltaic devices.

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