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Structural and Optical Studies of 100 MeV Ni^{+7} Irradiated Cadmium Selenide Thin Films

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The effect of irradiation with Swift (100 MeV) Ni^{+7} ions on the structural and optical properties of Cadmium Selenide (CdSe) thin films have been investigated at different fluencies in the range of 1×10^{11}-1×10^{13} ions/cm^{-2}. The CdSe films on glass substrates were prepared by thermal evaporation. The structural and optical changes with respect to increasing fluence were observed by the means of X-ray diffraction (XRD), UV-VIS and Raman spectroscopy. After irradiating the films with Ni^{+7} ions XRD show the increased in peak intensity and crystallite size with increasing fluence. The UV-VIS-IR spectroscopy revealed that there is decrease in band gap energy of the films after irradiation with increasing fluencies. Raman spectrum for as deposited and irradiated films show two peak, one at 209 cm^{-1} and at 410 cm^{-1} which is assigned to the longitudinal optical (LO) phonon mode.

Keywords: CdSe thin films, Swift heavy ion irradiation, XRD, UV, Micro-Raman.

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1. INTRODUCTION

Cadmium Selenide (CdSe), a II-VI compound semiconductor has been constantly invested during recent years for both fundamental and practical importance [1-3]. CdSe is a promising photovoltaic material because of its high absorption coefficient and nearly optimum band gap energy for the efficient absorption of light and conversion into electrical power [4-5]. The synthesis of binary metal chacogenide of groups II-VI semiconductors in a nanoparticle form has been a rapidly growing area of research due to their important non-linear optical properties, luminescent properties, quantum-size effect and other important physical and chemical properties [6-8]. CdSe thin films have been prepared by using thermal evaporation under vacuum is a very convenient method for obtaining uniform films. Currently, swift heavy ion (SHI) irradiation of material has generated significant interest in the light of application of such material in high radiation zones [9]. SHI irradiation has been reported of CdSe / FTO thin films deposited by electro deposition method. After irradiating the films there is increase in grain size, decrease in band gap was observed from structural and optical analysis [10]. In view of this, an effort has been made to study the structural and optical property of the SHI irradiated (100 MeV Ni^{+7} ion) thermally evaporation CdSe thin films using XRD, UV-Vis and Raman spectroscopy.

2. EXPERIMENTAL DETAILS

CdSe thin films of thickness 200nm have been prepared from 99.95 % pure CdSe powder (Alfa Aesar) in a vacuum evaporation unit (HHV-12A4DU) at a pressure of 1×10^{-6} mbar on clean glass substrate. Swift Heavy ion (SHI) irradiation of the as deposited CdSe films was done using 15 UD pelletron accelerator at Inter University Accelerator Center (IUAC), New Delhi, with 100 MeV Ni^{+7} at fluences levels 1.0×10^{11}, 1.0×10^{12} and 1.0×10^{13} cm^{-2}. The beam current was maintained at 2 pnA (particle nanoampere) during irradiation.

The focused ion beam was scanned over an area of 1 cm^2 using a magnetic scanner to achieve the fluence uniformity across the sample surface. The electronic and nuclear energy loss value for 100 MeV Ni^{+7} ions in CdSe, from the SRIM code simulation program (version 2003.26) are estimated to be 1.88×10^{1} eV/Å and 3.17×10^{-2} eV/Å respectively. The structural analysis of films was studied by X-ray diffractometer (Model JEOL 8030, $\lambda = 0.1541$ nm). The optical absorption spectra of CdSe thin films were obtained by a UV-VIS-NIR spectrophotometer in the wavelength range of 250 to 2500 nm. Micro-Raman spectroscopy was performed using Horiba Jobin Yvon Raman Spectrometer (T64000) and measurements were performed at room temperature with a 514.5 nm line of an Ar^+ laser.

3. INTERPERTATION OF EXPERIMENTAL RESULTS

3.1 X-ray Diffraction Studies

The X-ray diffractogram of pristine and irradiated CdSe thin films are shown in Fig. 1, a sharp peak in XRD pattern is observed in all the films oriented in (002) plane correspond to the hexagonal phase [11]. After irradiation the films have the same orientation and it was observed that after irradiation the intensity of the peak increases with increasing fluence. Such result have been observed for the CdSe films irradiated by Au^{8+} ions with energy of 100 MeV [10].

The effect of irradiation with increasing fluencies is summarized in Table 1. The grain size (D) is calculated for peak at $2\theta = 25.40°$ using the Scherer formula from the full-width half-maximum (FWHM) (β):

$$D = 0.94\lambda / (\beta \cos\theta), \quad (1)$$

where λ is the wavelength of X-ray used, θ is the half the angle between incident and the scattered X-ray beam. It is observed that the grain size increases with the increasing fluencies which indicate improvement in crystallinity.

The strain value (ε) can be evaluated by using the following relation:

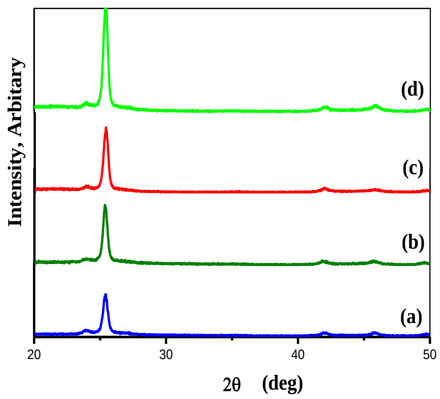

Fig. 1 – X-Ray diffractogram of pristine and SHI irradiated thin films of CdSe (a) Pristine (b) 1×10^{11} (c) 1×10^{12} (d) 1×10^{13} cm

$$\varepsilon = \beta \cos\theta / 4 \qquad (2)$$

The dislocation density (δ) has been calculated by using the following formula

$$\delta = 15\beta \cos\theta / 4aD \qquad (3)$$

The lattice spacing (d) is calculated from the Bragg's formul

$$d = \lambda / 2\sin\theta \qquad (4)$$

By this study it was observed that strain and dislocation density in the film decreases with the increases with fluencies [12].

Table 1 – Structural parameters of CdSe films irradiated at various fluences

Sample	2θ	Lattice spacing D [Å]	Grain size D [nm]	δ [$\times 10^{14}$] lines/m^2	Strain ε [$\times 10^{-3}$]	hkl
Pristine	25.40	3.504	27	15.34	1.737	002
1×10^{11}	25.37	3.508	42	12.57	1.182	002
1×10^{12}	25.35	3.510	56	9.43	0.753	002
1×10^{13}	25.32	3.513	69	7.26	0.474	002

3.2 UV-VIS Spectroscopy Studies

The transmission spectra of the as grown and irradiated CdSe film at different fluencies was measured in the wavelength range 250 to 2500 nm. The absorption coefficient (α) was calculated from transmission spectra in order to calculate the band gap (E_g). It is observed that E_g value decreases with increasing fluencies as shown in Fig. 2. Decrease in band gap energy which, in turn, depends on the increase of grain size of the CdSe films with increasing fluencies. The decrease in band gap energy of high-energy irradiated sample leads to ionization of atom, due to which change in the local structure order of films, as well as it induce lattice damage and creates defect energy levels below conduction band [13].

3.3 Raman Spectroscopy Studies

Fig. 3 shows the Raman spectra of as deposited and irradiated CdSe films at increasing fluencies. Raman

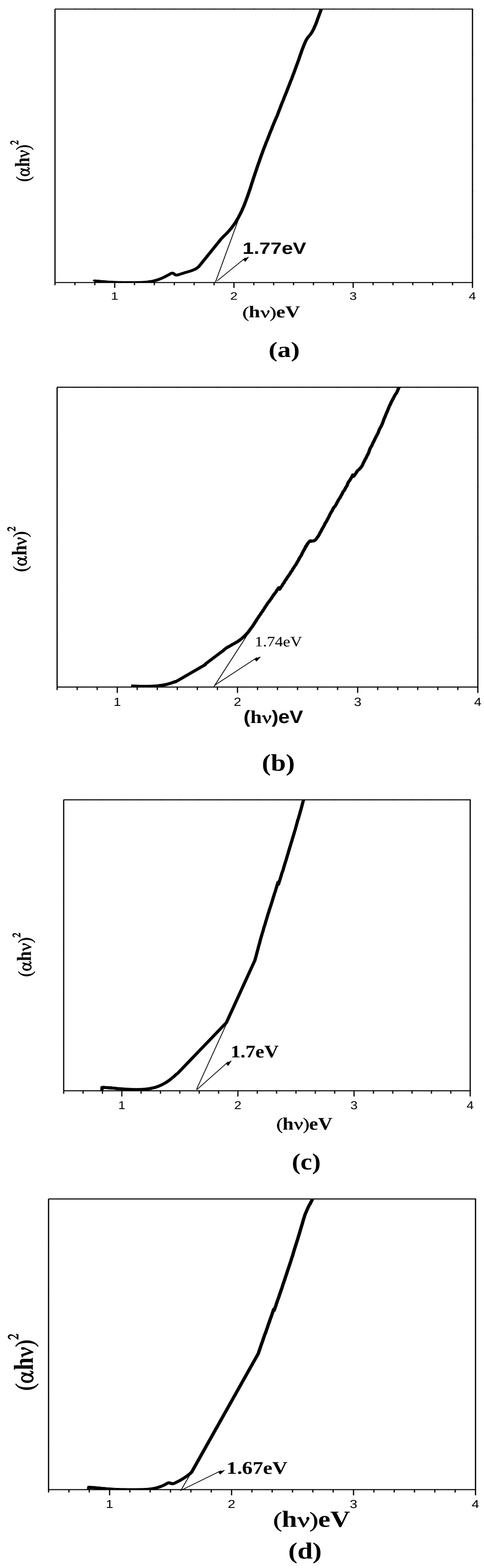

Fig. 2 – Variation of $(\alpha h\nu)^2$ against $(h\nu)$ for Pristine and SHI irradiated thin films of CdSe (a) Pristine (b) 1×10^{11} (c) 1×10^{12}, (d) 1×10^{13} cm^{-2}

spectrum for as deposited and irradiated films show two peak, 1LO and 2LO Raman peak at 209 cm^{-1} and 416 cm^{-1}. Second overtone of LO phonon mode is observed with decreasing intensity and also it was observed that intensity of Raman peak increases with increase in ion fluence. It is well known that the higher the intensity of the overtone, the better crystalline structure of the films [14]. Thus Raman spectra confirm formation of nanocrystalline CdSe thin films.

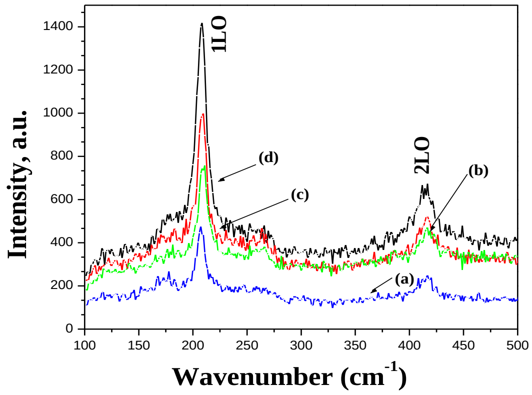

Fig. 4 – Micro-Raman spectrograph of thin films of CdSe Pristine and SHI irradiated (a) Pristine, (b) 1×10^{11}, (c) 1×10^{12}, (d) 1×10^{13} cm^{-2}

4. CONCLUSION

CdSe thin films deposited on glass substrate were irradiated using Ni^{+7} ions with energy of 100MeV at different fluences of 1.0×10^{11}, 1.0×10^{12} and 1.0×10^{13} cm^{-2} has been investigated using XRD analysis, UV-VIS-Spectroscopy and Micro-Raman spectroscopy. CdSe thin a film exhibits a hexagonal structure highly oriented with (002) plane. The grain size increases with increasing fluences. With the increase in fluences the average crystallite size increased whereas optical band gap decreased. Raman spectra measurements showed the presence of LO and 2LO phonon peaks.

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