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Structure and Surface Analysis of SHI Irradiated Thin Films of Cadmium Telluride

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Cadmium Telluride (CdTe) thin films grown by thermal evaporation on quartz substrates were irradiated with swift (100 MeV) Ni^{+4} ions at various fluences in the range $10^{11} - 10^{13}$ cm^{-2}. The modification in structure and surface morphology has been analyzed as a function of fluence using XRD and AFM techniques. The XRD showed a reduction in peak intensity and grain size with increasing fluence. The AFM micrographs of irradiated thin films show small spherical nanostructures. In addition to direct imaging, AFM profile data enable to derive the Power Spectral Density (PSD) of the surface roughness. In the present work PSD spectra computed from AFM data were used for studying the surface morphology of films. The PSD curves were fitted with an appropriate analytic function and characteristic parameters were deduced and discussed in order to compare film morphology with varying fluence levels.

Keywords: CdTe, Thermal Evaporation, Swift Heavy Ion Irradiation, XRD, AFM, PSD.

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1. INTRODUCTION

Cadmium telluride (CdTe), a II-VI compound semiconductor material, has high absorption coefficient, optimum bandgap, high stability and high efficiency suitable for photovoltaic applications [1]. The structure and surface morphology of the materials play crucial role for their use in practical thin film devices. Currently the swift heavy ion (SHI) irradiation of materials has generated significant interest in the light of application of materials in high radiation zones. SHI irradiation on CdTe crystal [2] and on thermally evaporated thin film of CdTe [3] to study the modification in the composition, structure and surface morphology as a function of ion fluence has been reported. CdTe thin films deposited by spray technique, SHI irradiated at various fluence levels using Silver ion [4] and Oxygen ion [5] has been reported. No significant work has been reported for surface analysis, using power spectral density on irradiated thin films of CdTe. In the present work, we investigate the structure and surface morphology of the SHI irradiated (100 MeV Ni^{+4} ion) thermally evaporated CdTe thin film using XRD & AFM techniques.

2. EXPERIMENTAL DETAILS

CdTe thin films of high purity and 100 nm thickness were deposited onto quartz substrates by vacuum evaporation from a molybdenum boat at a pressure of 5.0×10^{-7} mbar. Swift Heavy ion (SHI) irradiation of the as deposited CdTe films was done using 15 UD Pelletron accelerator at Inter University Accelerator Centre (IUAC), New Delhi, with 100 MeV Ni^{+4} for fluence levels 1.0×10^{11}, 5.0×10^{11}, 1.0×10^{12}, 5.0×10^{12} and 1.0×10^{13} cm^{-2}. The beam current was maintained at 2 pnA (particle nanoampere) during irradiation. The ion beam was focused to a spot of 10 mm diameter and scanned over an area of 1 cm^2 using a magnetic scanner to achieve the fluence uniformity across the sample area. The ladder current was integrated with a digital current integrator and the charged pulses were counted using scalar counter. The electronic and nuclear energy loss values for 100 MeV Ni^{+4} ions in CdTe, estimated from the SRIM code simulation program (version 2003.26) are 1.2516×10^3 eV/Å and 2.7181×10^3 eV/Å respectively.

The irradiated films were studied by X-ray diffraction technique using CuKα radiation. AFM measurements on the pre and post-irradiated thin films were performed with diInnova from Veeco Instruments. The quantitative analyses were carried out using Veeco software. All the AFM measurements have been performed in tapping mode (for both trace and retrace information) using a silicon nitride tip at ambient temperature.

3. RESULTS AND DISCUARTICLE STRUCTURE SSION

3.1 X-Ray Diffraction (XRD) Studies

Figure 1 shows the X-ray diffractogram of the pristine and irradiated CdTe thin films. As deposited CdTe films are oriented in the (111) and (311) planes in cubic phase. After irradiation films are found to be oriented in the same planes as of pristine. The lattice constant is found to increase with the increase in fluence. The lattice expansion might be due to modification of strain in the grains [5]. The grain size is found to decrease with increase in fluence which is in agreement with the result observed for 100 MeV Ag ion irradiation on thin film of CdTe (2). The decrease in peak intensity and the increase in the peak width are observed with increase

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in fluence. These changes are attributed to the reduction in crystallinity of the material, formation of point defects, defect clusters, additional grain boundaries and amorphization of the film.

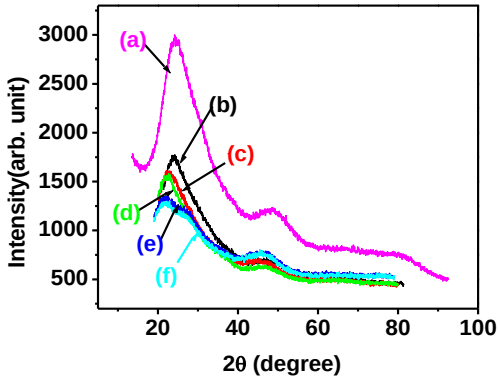

Fig. 1 – X-Ray Diffractogram (a) Pristine (a), 1.0×10^{11} (b), 5.0×10^{11} (c), 1.0×10^{12} (d), 5.0×10^{12} (e), 1.0×10^{13}cm^{-2} (f)

Table 1 – Variation of FWHM, lattice constant and strain

Fluence (ions-cm^2)	FWHM (degree)	d (Å)	a (Å)	Strain
Pristine	8.2498	3.5500	6.1497	2.013
1×10^{11}	4.1974	3.6897	6.3909	1.026
5×10^{11}	4.0574	3.7574	6.5080	0.993
1×10^{12}	3.8229	3.7730	6.5352	0.938
5×10^{12}	3.6357	3.7902	6.5793	0.891
1×10^{13}	3.6112	3.8105	6.6015	0.886

3.2 Atomic Force Microscopy (AFM) Studies

The AFM image of the surface of the as-deposited film as shown in Figure (2a) is smooth and uniform and reveals that the grains are spherical and compactly packed. The surface of irradiated samples is seen to be different from that of the as-deposited film figure (2a). The AFM spectral analysis showed that on increasing the fluence, the CdTe atoms diffuse into the film surface to agglomerate and forms nanograin chains on the thin film surface figure (2c & 2d). On increasing the fluence, this process continues along with the increase in both the surface roughness and the density of the nanograin chains (figure 2(c), (d), (e)). The variation of average roughness (R_a) and RMS roughness (R_q) is shown in Table 1. It is seen that by increasing the fluence from 1.0×10^{11} cm^{-2} to 1.0×10^{12} cm^{-2} the R_q increases from 2.52 nm to 8.79 nm and then decreases to 2.05 nm for fluence 1.0×10^{13}cm^{-2}. However, the R_q of the as-deposited film was measured to be about 1.18 nm. This means that the irradiation transformed the as-deposited surface to nanostructured rough surfaces. With the increase in the fluence, predominance of surface diffusion over the surface tension of the thin films occurs. On increasing the fluence further, causes a slight decrease in the surface roughness. Each ion is expected to electronically sputter out material from the surface around a region surrounding the ion path. The surface density of the sputtered regions would thus scale with ion fluence (6). From fluence of 1.0×10^{11} cm^{-2} to 1.0×10^{12} cm^{-2} the increase in

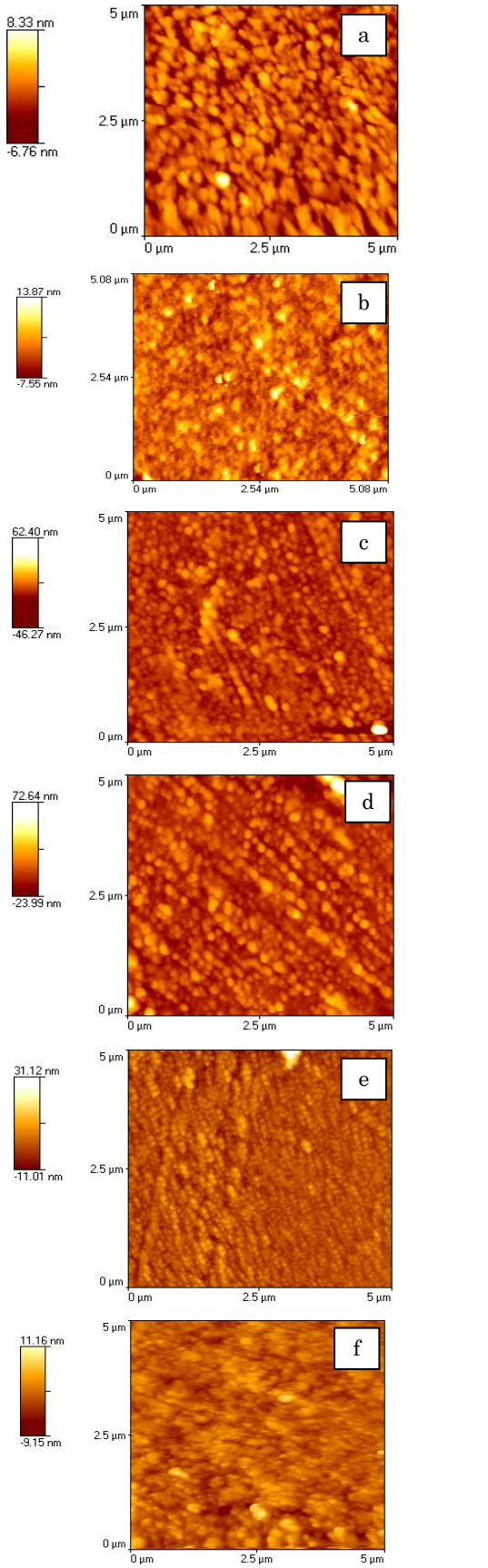

Fig. 2 – AFM micrographs of Pristine and irradiated films Pristine (a), 1.0×10^{11} (b), 5.0×10^{11} (c), 1.0×10^{12} (d), 5.0×10^{12} (e), 1.0×10^{13} (f)

Table 2 – Variation of Average roughness, rms roughness, and Average height obtained from AFM with fluence

Fluence	Average surface roughness R_a (nm)	Rms surface roughness R_q (nm)	Average height (nm)
Pristine	0.94	1.18	4.17
1.0×10^{11}	1.94	2.52	7.55
5.0×10^{11}	4.17	5.75	46.27
1.0×10^{12}	6.61	8.79	23.99
5.0×10^{12}	2.34	3.16	11.01
1.0×10^{13}	1.62	2.05	6.97

roughness seems to arise due to electronic sputtering by individual ions. With increasing fluence to $1.0 \times 10^{13}\,\mathrm{cm}^{-2}$ a decrease in roughness may arise due to the overlap of damaged zones. This overlap would lead to smoothening in heavily damaged surfaces. Thus at higher fluences, due to the intermixing process, average height of grains decreases which in turn results in the decrease in surface roughness as well.

3.2.2 Power Spectral Density (PSD) Analysis

The surface rms roughness will be insufficient to supply the complete information of the surface modifications and PSD is evaluated to provide quantitative information about the surface roughness both in the vertical and lateral directions. The PSD curves of pristine and irradiated CdTe thin films are shown in Figure 3. With in the frame- work of the k-correlation or ABC model, the auto-covariance function PSD_{ABC} for spatial frequency f, for a two-dimensional isotropically rough, self affine fractal surface with a crossover region is given by [6, 7]

$$PSD_{ABC} = (A)/(1 + B^2f^2)^{(C+1)/2},$$

where A, B and C are the function parameters.

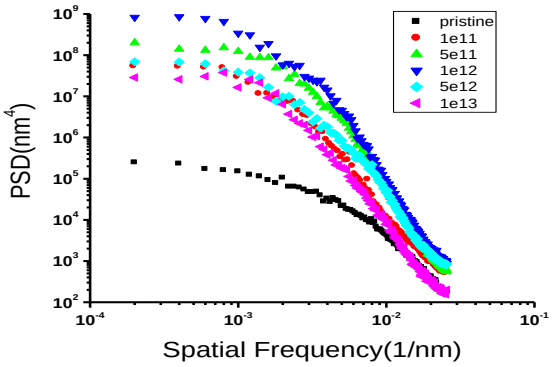

Fig. 3 – Power Spectral Density Vs Spatial Frequency plot of Pristine and irradiated Films

At small f values, well below the "knee" or the crossover region, the PSD is determined by A, which is related to the height of the surface roughness. At high f values, beyond the "knee", the surface is fractal and the PSD function is determined by C. PSD plot is fitted in this ABC model and the values of A, B, C are given in Table 2. The parameter A is higher for the fluence of $1.0 \times 10^{12}\,\mathrm{cm}^{-2}$, which corresponds to peak-to-valley

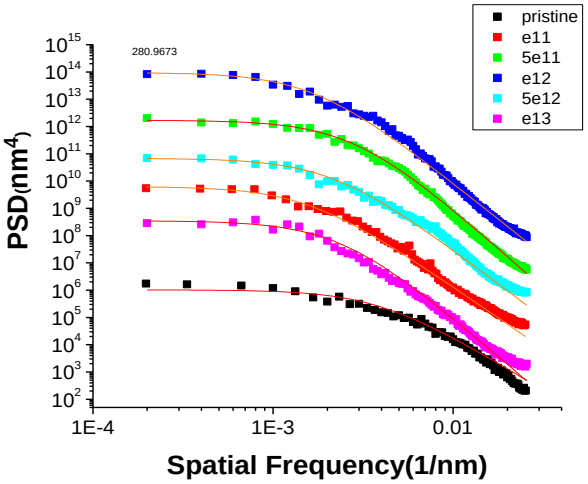

Fig. 4 – Power Spectral Density Vs Spatial Frequency plot of Pristine and irradiated Films with ABC Model fitting

Table 3 – Parameters for k correlation model for PSD plots

Fluence	A (nm^4)	B (nm)	C
Pristine	1.02×10^6	280.00	3.20
1.0×10^{11}	7.96×10^7	637.12	3.56
5.0×10^{11}	1.62×10^8	354.87	4.58
1.0×10^{12}	9.55×10^8	584.16	4.27
5.0×10^{12}	6.48×10^7	464.93	4.10
1.0×10^{13}	3.72×10^7	418.97	4.68

values. Grain size increases significantly for the fluence $1.0 \times 10^{11}\,\mathrm{cm}^{-2}$. For pristine sample the roughness is quite low. For fluence $1.0 \times 10^{11}\,\mathrm{cm}^{-2}$ roughness increases as compared to pristine up to a fluence $1.0 \times 10^{12}\,\mathrm{cm}^{-2}$ and then decreases up to the fluence of $1.0 \times 10^{13}\,\mathrm{cm}^{-2}$. In mid-frequency range, the crossover point (knee) of PSD plot corresponding to X-axis gives correlation length which is related to mean grain size. The **quantity B determines the position of the "knee", which** is related to the correlation length. The grain size for pristine is found to be 280 nm and it increase for the fluence $1.0 \times 10^{11}\,\mathrm{cm}^{-2}$ and then decreases for the fluence $5.0 \times 10^{11}\,\mathrm{cm}^{-2}$. Grain size decrease after the fluence level of $1.0 \times 10^{12}\,\mathrm{cm}^{-2}$. The value of parameter C, corresponds to the inverse slope of the PSD curve. It is reported that the film growth corresponding to the viscous flow, evaporation and condensation, bulk diffusion and surface diffusion shows the value of C as 1, 2, 3 and 4 respectively (7). Thus the CdTe thin films which were grown from thermal evaporation, shows surface diffusion after irradiation. The average height (Table 1) thus shows similar variation as rms roughness in case of all samples. As seen from the PSD in higher frequency range, plot for pristine is almost linear and shows ideal fractalness of the surface.

4. CONCLUSION

The CdTe films deposited on quartz substrates by thermal evaporation process have been investigated. The effect of SHI irradiation with varying fluence on the micro structural characteristics such as grain morphology and surface roughness of CdTe films have been analyzed. The experimental results have shown that the grain size reduces with increase in fluence. The surface

roughening is more for fluence of $1.0 \times 10^{12}\,\mathrm{cm}^{-2}$ and starts decreasing with increase in fluence. It is found that the nanograin chains are formed at fluence of $1.0 \times 10^{12}\ \mathrm{cm}^{-2}$. The AFM surface imaging with PSD analysis has been used to analyze the mechanism of growth and modification due to irradiation.

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