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Effect of 100 MeV (7+) Oxygen ion irradiation on the structural properties of Cadmium Telluride thin films

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Abstract: Polycrystalline Cadmium Telluride (CdTe) thin films were prepared using thermal evaporation method at 150 °C substrate temperature. These samples were irradiated with 100 MeV (7+) oxygen ions for various fluences namely 1×1011, 5×1011, 1×1012 and 5×1012 ions/cm2, to study the irradiation effects on structural properties. X-ray diffraction patterns showed increase in crystallinity and enhanced microstructure up to the fluence of 5×1011 ions/cm2. For higher fluences 5×1012 ions/cm2, microstructure and surface morphology decreases which is an advantages as it increases the efficiency of the CdTe solar cells. The detailed studies have been presented and discussed in this paper.

Keywords: CdTe, Thermal evaporation, Ion Irradiation, Annealing, Morphology

1. Introduction

Cadmium Telluride belongs to the family of II–VI compound semiconductors and exhibit many interesting solid-state phenomena of considerable practical importance. CdTe is a direct band gap (1.54 eV) material used in radiation environments such as reactors and space applications. CdTe is also used in the fabrication of advanced infrared detectors for satellite based surveillance, solar cells, X-ray detectors, gamma ray detectors and other important applications [1–5]. The irradiation effect of energetic heavy ions on the structure of the materials used for space applications is a further stimulating aspect. In the outer space, electronic devices are exposed to cosmic radiations, comprising a variety of high energy particles, which may degrade their performance over years of operation.

2. Experimental

CdTe thin films were deposited on chemically cleaned glass substrates using a conventional vacuum coating unit (Hind High Vacuum Company, Bangalore Model 12A4D). The starting material (99.999% pure stoichiometry CdTe powder from Sigma Aldrich) was evaporated from a molybdenum boat at a pressure of 1 ×10–5 mbar. The thickness of the film was monitored in situ by quartz crystal thickness monitor and is about 1 µm. Ion beam irradiation was carried out using 15 UD Pelletron tandem accelerators. Films of 1 cm2 area were mounted on a ladder in an irradiation chamber evacuated at a pressure of 10–6 mbar. The films were subjected to 100 MeV oxygen (7+) ion radiations for different fluences namely 1×1011, 5×1011, 1×1012 and 5×1012 ions/cm2. The beam current was maintained 1 pnA (particle nano-ampere) to avoid heating effect during irradiation. The ion beam was focused to a spot of 10 mm diameter and then scanned over an area of 1 cm2 using magnetic scanner to achieve the dose uniformity across the sample area. The fluence values were measured by collecting the charge falling on the sample mounted on an electrically insulated sample ladder placed in secondary electron suppressed geometry. Ladder current was integrated with a digital current integrator and the charged pulses were

counted using scalar counter. The films were characterized before and after irradiation to study the influence of irradiation on the film properties.
The un-irradiated and irradiated samples are characterized using Bruker (AXSD8 Advance) X-ray diffractometer with Cu Kα radiation having a wavelength of 1.5406 Å as the X-ray source. The morphological studies were carried out using a Multimode IIIa, Digital Instruments atomic force microscope.

3. Result and discussion.

Structural Properties

X-ray diffractogram of the un-irradiated and irradiated CdTe thin films is shown in Fig. 1. CdTe deposited in cubic zinc blend structure, preferably oriented along (111) plane. SHI irradiation can be explained by total energy deposited in electronic excitations/ionizations of respective CdTe atoms in the films by energetic ions. The range of 100 MeV oxygen ions in CdTe was calculated using TRIM [22] and is found to be 64.45 µm. Since CdTe thin films are about 1 µm thick it can be assumed that ions penetrated the thin films with an almost constant value of electronic energy loss Se = 112.030 eV/Å. It can be noticed that intensity of peaks increases with irradiation and is maximum for the sample irradiated to 5×1011 ions/cm2. This increase in intensity is indication of improvement in crystallinity due to the annealing of defects at a low fluence [11, 18, 21]. However, for further increase in the ion fluence, peak intensity decreases slightly due to the formation of point defects, defects clusters, partial amorphization [11, 23]. The increase and decrease of diffraction intensity could be expected on the irradiated films due to creation or annihilation of defects and recrystallization.

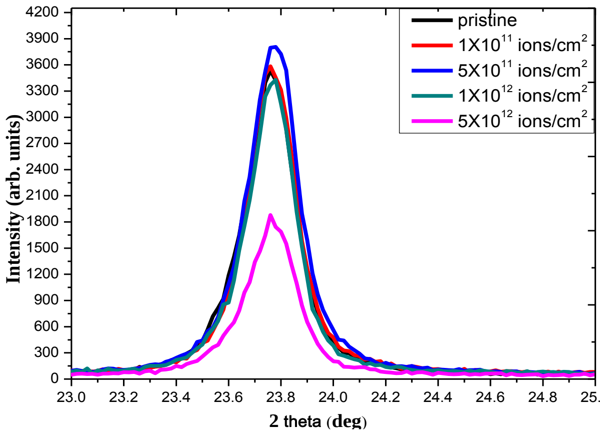

Figure 1 : X-ray diffractogram of un-irradiated and irradiated CdTe thin films.

Shift in diffraction peaks towards lower diffraction angle from its corresponding powder data [2θ=24.026 degrees JCPDS number 75-2086] indicates the developments of tensile tress in the as-grown film [2θ = 23.779 degrees]. Displacement of diffraction peaks is an indication of development of tensile stress normal corresponding to crystal plane in the film during condensation. The films grown by any technique will have a tensile stress of certain magnitude depending on the material and growth conditions. The value of tensile stress is calculated by multiplying the strain produce, using the equation,

$$\frac{\Delta d}{d} = \frac{d(observed) - d(ASTM)}{d(ASTM)} \times C11 \qquad (1)$$

Where, C11=5.351×1010 Pa, is the elastic stiffness constant of CdTe and ASTM stands for American Society for Testing of Materials.

Fig. 2. illustrates the variation of tensile stress as a function of ion fluence. There are many structural transformations that may influence on the stress in a film like creation of hillocks, shrinkage of grain boundary voids are amorphization of the films or substrate. It is very difficult to determine the exact physical process, which caused the changes of residual tensile stress. Samples have small stress and there is no much change in the stress after irradiation. The complete structural analyses of the films were given in the Table 1. It can be noticed from the table1 that dislocation density is increased in the sample irradiated to highest fluence which indicates the change in the microstructure of the film due to ion irradiation.

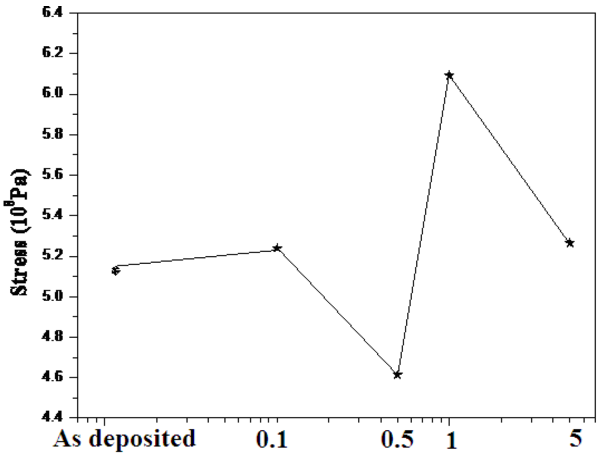

Figure 2 : Variation of stress with fluence (1012 ions/cm2)

Table 1 : Microstructure analysis of the 100 MeV oxygen irradiated CdTe thin films

Irradiated Sample (ions/cm^2)	Lattice constant d (Å)	Grain size D (Å)	Dislocation density ($\times10^{14}$) (lin/m^2)	Stress ($\times10^8$ Pa)
CdTe -as deposited	6.47572	478.4827	4.36785	5.13
1×10^{11}	6.47732	474.775	4.36794	5.24
5×10^{11}	6.46985	478.502	4.3675	4.61
1×10^{12}	6.48489	478.444	4.36855	6.10
5×10^{12}	6.47766	430.6285	5.39255	5.26

Average grain size of un-irradiated and irradiated samples were calculated using the Debye-Scherer formula, D = 0.9λ/(β Cosθ), where, D is the diameter of crystallites forming the films, λ is the wavelength of X-ray source, β is Full Width Half Maximum [FWHM] in radiance and θ is the Brag angle. Dislocation densities present in the samples were calculated as □= 1/D2 and presented in the table 1.Grain size increases maximum for the sample irradiated to 5×1011 ions/cm2 and decreases for the sample irradiated to 5×1012 ions/cm2. This variation in the grain size is due to the ion beam induced recrystallization. The average grain/particle size before irradiation was 478.45 Å, which upon irradiation at fluence 5×1012 ions/cm2 decreases to 430.62 Å, as calculated by Scherrer's equation.

Surface Morphology

Parameter of easy physical interpretation used to characterize the surface morphology of thin films is its roughness, which can be considered as an inheritance of growth process. The measured RMS roughness for 1×1 micrometer area of the as grown sample and samples irradiated to ion fluence of 5×1011 and 5×1012 ions/cm2 is 4.782, 4.553 and 5.019 nm respectively.

Fig. 3. shows the three dimension AFM images of CdTe film surface before and after irradiation. RMS roughness increases for the irradiated sample due to the increase in dislocations and cracks created by the oxygen irradiation. After irradiation the grains seem to be more closely packed due to melting of grains followed by re-growth, which is clearly seen from Fig. 3b and 3c. Increase in the surface roughness is advantages as it increases the efficiency of the CdTe solar cells [25].

4. Conclusion

CdTe thin films prepared using thermal evaporation method were irradiated with 100 MeV oxygen ions for different fluences. There is a significant change in the material characteristics because of influence of energetic ions. The study highlights the change in the stress in the samples due to irradiation. Changes in the morphology of the films were also noticed in the irradiated thin films. The morphology of the irradiated films reveals increase in surface roughness, which is more desirable to enhance the solar cell efficiency.

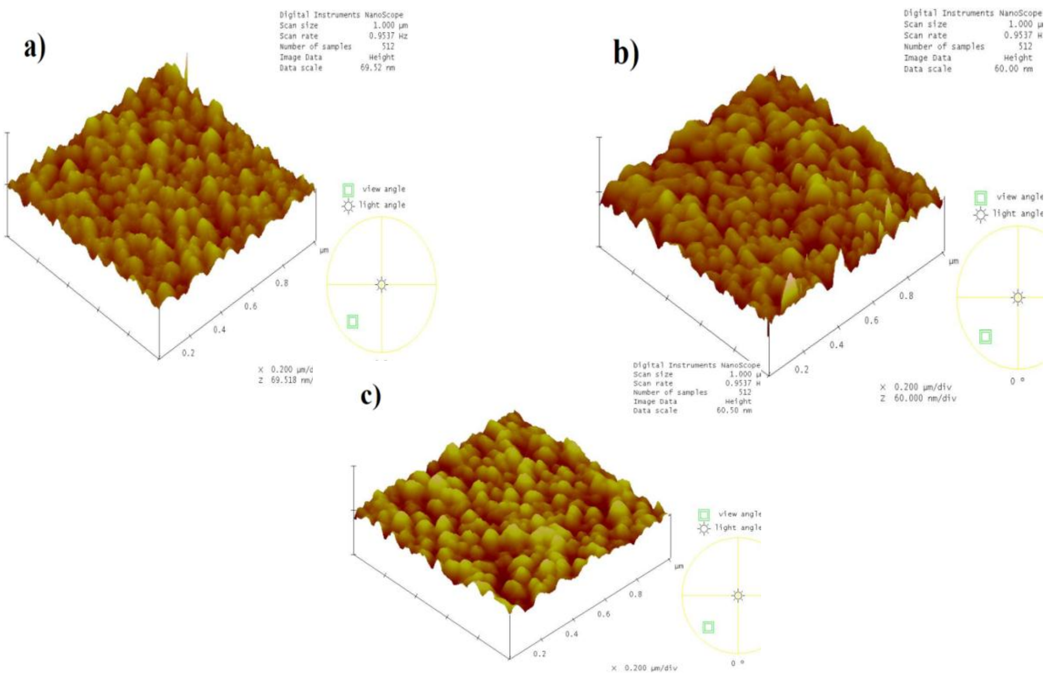

Figure 3 : AFM graphs of a) as-deposited b) 100 MeV oxygen irradiated CdTe thin films for the fluence 5×10^{11} and c) for 5×10^{12} ions/cm^2

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