

An effect of Ar⁺ ion irradiation on structural and optical properties of electron beam evaporated Cadmium Telluride thin films

S. SHANMUGAN*, D. MUTHARASU

Nano Optoelectronics Research Laboratory, School of Physics, Universiti Sains Malaysia, 11800, Penang, Malaysia

CdTe thin films were prepared using e-beam evaporation technique. The prepared films were irradiated by Ar⁺ ion at different fluency using Multipurpose Al probe as insitu. This could be also used for ion bombardment for cleaning the substrate prior to coating. The prepared and ion irradiated films were confirmed as polycrystalline nature with X-ray technique. From the results, Ar⁺ ion irradiation enhanced the (111) orientation of CdTe crystals. A considerable modification on structural parameters like crystallite size, lattice parameter, internal strain etc. could be observed as a result of high Ar⁺ ion fluency. The observed band gap was increased for higher Ar⁺ ion fluency. It shows the effect of Ar⁺ ion irradiation in the modifications of optical properties. The observed results were encouraging on the use of simple multipurpose Al probe for Ar⁺ ion irradiation process as insitu.

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1. Introduction

In the recent years, thin films are much interest because of their various applications in semiconducting devices, photovoltaic's, optoelectronic devices, solar energy converters etc. [Chandramohan et. al. 2004, Deshmukh et al. 2005]. Ion bombardment plays an important role on the film properties such as crystallinity, packing density, surface roughness, etc. [Tominaga et. al. 1996]. Parish et al 1986 have studied the lattice disorder produced in CdS crystals on implantation with different types of ions. If the semiconductor is implanted with electrically inactive ions then the resultant effects can be attributed exclusively to the lattice disorder. The modification on the optical band gap and the absorption coefficient have been observed from the Ar⁺ and N⁺ ion implanted CdS thin films and also the formation of Cd metallic clusters have been reported elsewhere [Senthil et. al. 2002]. Normally ion irradiation process had been carried out by using separate ion sources in a separate vacuum chamber. It may affect the properties of thin films as well as the device while transit for process after deposition. Shanmugan et al 2009 have tried to irradiate the O⁸⁺ ion generated by simple multipurpose Al probe to study the influence on structural and optical properties of e-beam evaporated CdTe thin films. In the present work, e-beam evaporated CdTe thin films were irradiated by Ar⁺ ions as *in-situ* using multipurpose Al probe located at inside the vacuum chamber and the effect of Ar⁺ ion fluency on the structural and optical properties are reported here.

2. Experiment

CdTe thin films were deposited over the glass substrate by E-beam evaporation technique. To get the

uniform film thickness, rotary drive assembly was used and all films were coated with constant speed of 40 rpm. Prior to coating, the substrates were cleaned by O⁸⁺ ion bombardment process in presence of high pure O₂ using multipurpose Al probe which is followed by conventional cleaning. The probe has the surface area of 49.5 cm². The substrate –source distance was fixed at 14 cm. The CdTe thin films with 240 nm thickness were prepared under the vacuum of 7×10^{-6} mbar. The rate of deposition was maintained at 2Å/sec.

The Ar⁺ ion irradiation processes was performed for about 10 minutes with three different ion flux densities (3.14×10^{16} ions/cm² sec, 6.294×10^{16} ions/cm² sec and 9.44×10^{16} ions/cm² sec) in presence of ultra high pure Ar gas. The chamber pressure of about $2 - 5 \times 10^{-3}$ mbar was maintained for all ion irradiation process. The flux densities were fixed by adjusting both Al probe current and gas pressure inside the chamber. The distance between the probe and substrate was fixed as 6 cm. The structural properties were analyzed by XRD technique using Cu-K α radiation ($\lambda = 1.5406 \text{ \AA}$) in Bruker D8 Advance diffractometer. The transmittance spectra were recorded using a double beam Shimadzu UV 160A Spectrophotometer in the wavelength range from 400 to 1100 nm.

3. Results and discussions

3.1 Structural properties

An Ar⁺ ion irradiated CdTe thin films were analyzed with XRD technique and the observed spectra is shown in Fig. 1(a). It shows that the intensity of preferred (111) oriented peak gets increases and also the intensity of (220) and (311) peaks get decreases as with Ar⁺ ion doses increases. It can also be observed that the Ar⁺ ion flux

helps to increase the crystallinity of the films which may be attributed to the reduction of Cd vacancy [Rusu et al 2005]. It seems that the Ar^+ irradiation with higher fluency supports to grow the crystalline CdTe thin films. To

understand in detail, the structural parameters were calculated from the XRD spectra (see Table 1) and discussed in the consecutive section.

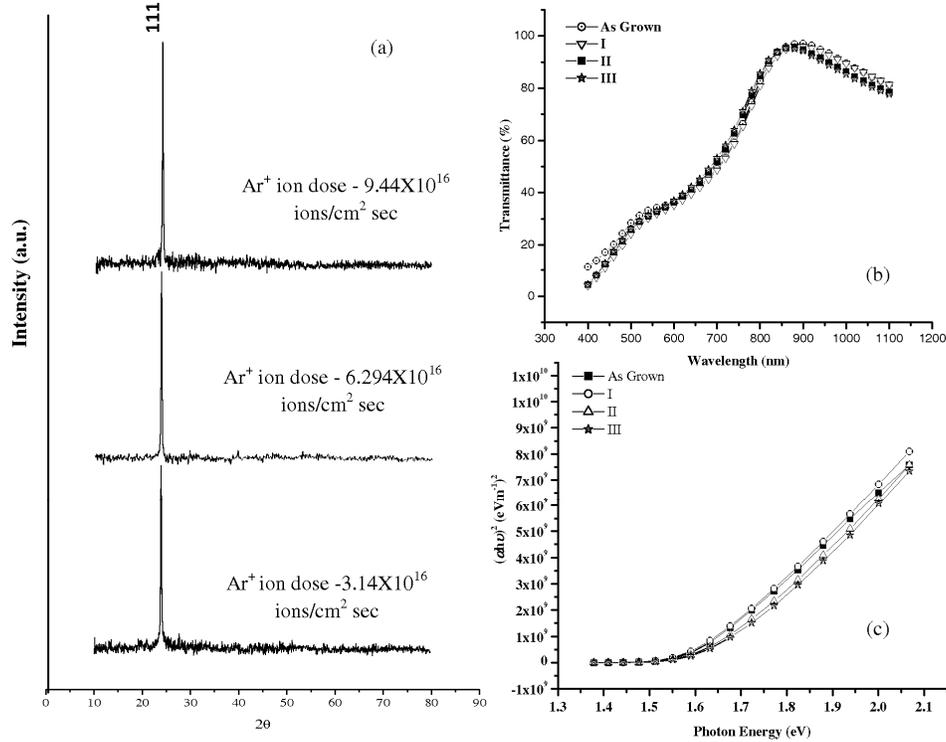


Fig. 1. XRD pattern (a), Transmittance (b) and Bandgap (c) of Ar^+ ion irradiated CdTe thin films prepared by ebeam technique.

The crystallite size (D) was calculated using the Debye Scherer formula [Gordillo et al 1995] from the full-width at half-maximum (w) measurements:

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

The strain (ε) was calculated from formula

$$\varepsilon = w \cos\theta / 4 \quad (2)$$

The dislocation density (δ), defined as the length of dislocation lines per unit volume of the crystal, was evaluated from the relation [Williamson et al 1956]

$$\delta = 1 / D^2 \quad (3)$$

The lattice parameter ' a ' was evaluated from the expression

$$a^2 = d^2 (h^2 + k^2 + l^2) \quad (4)$$

where h, k, l are Miller indices. The internal stress (σ) in the deposited film is calculated using the relation

$$\sigma = -E (d_a - d_o) / (2d_o Y) \quad (5)$$

where d_o and d_a are the d spacing of CdTe bulk and thin film form respectively. E and Y are the Young's modulus and Poisson's ratio of CdTe respectively [Perry 1990].

From the Table 1, it is observed that the crystallite size decreases from 7.52 nm (as grown) to 4.93 nm (irradiated) as with Ar^+ ion dose increases. The increase in crystallite size seems to be the formation of higher dislocation density in the irradiated films. In addition to that, the calculated lattice parameter is decreased considerably as with Ar^+ ion fluency. It is due to the formation of dense crystallites as a result of cell volume contraction. The observed lattice constant of Ar^+ ion irradiated CdTe thin films is less compared to that of the pure CdTe. A decrease in d space value also demonstrates the effect of Ar^+ ion irradiation clearly. Due to ion irradiation on the surface of the prepared films, there may be a change in the atomic vibration as a result of ion collisions at nearby the surface. This effect may develop the stress which is applied perpendicular to the thin film surface.

The sign of the internal stress observed from the calculation reveals the nature of stress applied on the film surface. In Ar^+ ion irradiation process, the nature of stress is applied is as tensile since the results show the negative

sign in Table 1. It is observed that the applied tensile stress of Ar⁺ ion irradiated thin films is comparatively more than that of as grown samples. A noticeable effect on micro

strain could also be observed for various Ar⁺ ion fluency and reported as increases with ion fluency.

Table 1. Structural parameters of Ar⁺ ion irradiated CdTe thin films.

Processing parameter (ion irradiation)	Internal stress σ (GPa)	d space (\AA)	Lattice constant (a)	Micro strain ϵ ($\times 10^{-2} \text{ lin}^{-2} \text{ m}^{-4}$)	Dislocation density δ ($\times 10^{18} \text{ lin/m}^2$)	Crystallite size D (nm)
As grown	-0.09675	3.7361	6.4709	4.814	1.77	7.52
Pro.I + Ar ⁺ ion	-0.27575	3.7256	6.4536	7.338	4.11	4.934
Pro.II + Ar ⁺ ion	-0.39907	3.7184	6.440	7.262	4.02	4.985
Pro.III + Ar ⁺ ion	-0.22621	3.7285	6.4571	7.338	4.11	4.934

3.2 Optical properties

In order to study the effect of Ar⁺ ion irradiations on the optical behavior, transmission spectra were recorded for all samples and shown in Fig. 1(b). It shows that the Ar⁺ ion fluency does not affect the transmission curve considerably. But the presence of small interference curve reveals the uniform film thickness even after ion irradiation process. Variation in bandgap with respect to the photon energy is represented in Fig. 1(c). It shows that the band gap value increases with Ar⁺ ion fluency increases.

The absorption coefficient (α) was calculated from the transmittance spectra using the relation

$$\alpha = 4\pi k_f / \lambda \quad (6)$$

The optical band gap of all films were analyzed using the relation

$$ah\nu = A (h\nu - E_g)^{1/2} \quad (7)$$

where A is a constant.

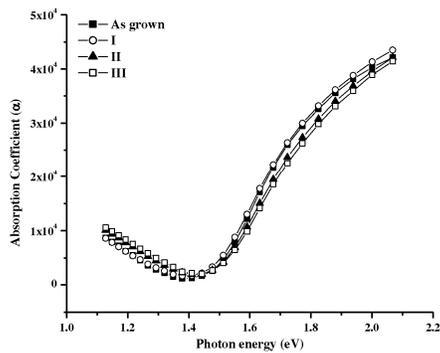


Fig. 2. Absorption coefficient of Ar⁺ ion irradiated CdTe thin films.

The observed band gap value lies between 1.55 (as grown) and 1.62 eV (for higher Ar⁺ ion doses). The calculated absorption coefficient is plotted against the photon energy in Fig. 2. It shows that there is no considerable influence on the absorption coefficient could be observed for various Ar⁺ ion fluency.

4. Conclusion

E-beam evaporated CdTe thin films were irradiated with Ar⁺ ions produced by simple multipurpose Al probe. The structural analysis state the possibility in the formation of preferred oriented CdTe thin films by Ar⁺ ion irradiation as *in situ* process. The irradiation process also helps to modify the structural parameters for various ion fluencies. From the observed optical properties, it is concluded that Ar⁺ ion irradiation helps to improve the band gap of the prepared CdTe thin films as well as the other structural parameters.

References

- [1] R. Chandramohan, T. Mahalingam, J. P. Chu, P. J. Sebastian. Sol. Energy Mater. Sol. Cells. **81**, 371 (2004).
- [2] S. K. Deshmukh, A. V. Kokate, D. Sathe, J. Mater. Sci. Eng. B **122**, 206 (2005).
- [3] K. Tominaga, S. Inoue, R. P. Howson, K. Kusaka, T. Hanabusa. Thin Solid Films **281**, 182 (1996).
- [4] N. R. Parish, D. A. Thompson, G. J. C. Carpenter. Radiat. Eff. **98**, 289 (1986).
- [5] K. Senthil, D. Mangalaraj, Sa. K. Narayandass, B. Hong, Y. Roh, C. S. Park, et. al, Semicond. Sci. Technol. **17**, 97 (2002).
- [6] S. Shanmugan, S. Balaji, D. Mutharasu, N. Sankarasubramanian. International Journal of Micro and Nano system, **1**, 29 (2009).
- [7] G. G. Rusu, M. Rusu, J. Optoelectron. Adv. Mater. **7**, 885 (2005).
- [8] G. Gordillo, J. M. Flez, L. C. Hernandez. Sol. Energy Mater. Sol. Cells **37**, 273 (1995).
- [9] G. B. Williamson, R. E. Smallman III. Philos. Mag. **1**, 34 (1956).
- [10] A. J. Perry, J. Vac. Sci. Technol. **A 8**, 1351 (1990).

*Corresponding author: subashanmugan@gmail.com