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Effect of annealing temperature on grain growth of nanocrystalline CdTe thin films

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Abstract: CdTe thin films of varying thickness of 100nm, 200 nm and 300 nm each are deposited by vapor deposition technique and later annealed at 400°C in argon. The phase determined by XRD reveals that the grain size of CdTe phase is strongly dependent on the film thickness and is found to increase with the film thickness. The Raman spectrum shows peaks corresponding to CdTe and the intensity of Raman peaks is found to decrease with increasing grain size. The elemental composition of all the films is studied by EDAX and shows nearly stoichiometric composition of Cd and Te but slightly excess of Te has been reported.
Keywords: Effect of annealing temperature, grain growth, nanocrystalline CdTe thin films.

Introduction:

CdTe is extensively used semiconductor in fabrication of devices. It is the most preferred material for low cost solar cell application due to its high optical absorption coefficient for visible spectrum and nearly optimum band gap[1]. CdTe thin films deposited by several techniques like spray pyrolysis[2], electro deposition[3], closed space sublimation[4], vacuum evaporation method[5] have been investigated for obtaining device grade CdTe thin films. It becomes essential to understand the microstructure and morphology evolution of CdTe films as this affects performance of active devices such as solar cells fabricated from these layers. The grain size and surface morphology are often defined during the film growth period which could be tempered through high temperature annealing post deposition[6]. The efficiency conversion of thin film CdTe device is strongly dependent on the structural, optical and electrical properties[6]. In this work, CdTe thin films of varying thickness are deposited on a fused silica substrate and are annealed to at 400°C. Effects of the post deposition annealing on the film properties such as grain size; phase formation and elemental content are discussed.

Experimental:

CdTe films are deposited on fused silica substrates (1cm x 1cm x 1mm) by vacuum evaporation technique by evaporating 99.99% CdTe powder. The films are deposited at three thickness namely 100 nm, 200 nm and 300 nm. These films are annealed at 400°C in argon atmosphere. Argon is chosen as the ambient as to avoid contamination from the air atmosphere resulting in formation of native oxide layer. The post deposition annealed films are characterized by X-ray diffraction and Raman spectroscopy for phase formation studies and elemental composition is studied by Energy Dispersive X-ray analysis (EDAX). The XRD is performed using Cu-Kα radiation with λ= 1.5418 A on a Phillips Panalytical Xpert Pro MPD spectrometer. The samples were scanned for the 2θ of 20°-80° and were rotated at a speed of 0.0006°/Sec. EDX measurements are done by Oxford INCA PentaFET -x3 and Raman spectra is obtained by Reins haw In via Raman microscope.

Results and Discussions:

XRD Studies

X-ray diffraction (XRD) is used to determine the phase and structure of CdTe films. Fig 1 shows the XRD spectra of CdTe films of 100 nm, 200 nm and 300 nm deposited on to the quartz substrates and annealed at 400°C. The structure of all the three film shows peaks corresponding to hexagonal and cubic CdTe phases. The initiation of the formation of CdTe structure is observed with feature peaks at 2θ= 23.74, 39.38 and 46.48 corresponding to (111), (110), (102), planes of hexagonal and cubic CdTe as confirmed from JCPDS X-ray powder file data[7]. The diffraction intensity of CdTe peaks is found to be increasing with increasing annealing temperature due to the growth with annealing temperature[8]. For all the three thickness of the CdTe films, the peak intensity of (111) was high compared to other peaks. This indicates preferential orientation of the micro-crystallites is in (111) direction which is perpendicular to the surface[9]. The full width at half maximum (FWHM) of the cubic (111) peaks were calculated and was found to decrease with decrease in thickness. The decrease in FWHM could be attributed to decrease in the concentration of lattice imperfection as the micro-strain decreases within the film and the crystallite size increases. The grain size is calculated using Debye Scherrer formula for crystallite size $D = (0.94\ \lambda/\ \beta \cos\theta)$ where β is the full width half maxima in radians, λ is the wavelength of X-rays. The grain size is found to be 31 nm, 35 nm and 37 nm for films of thickness 100 nm, 200 nm and 300 nm respectively. It is noted that the grain size increases with increasing film thickness.

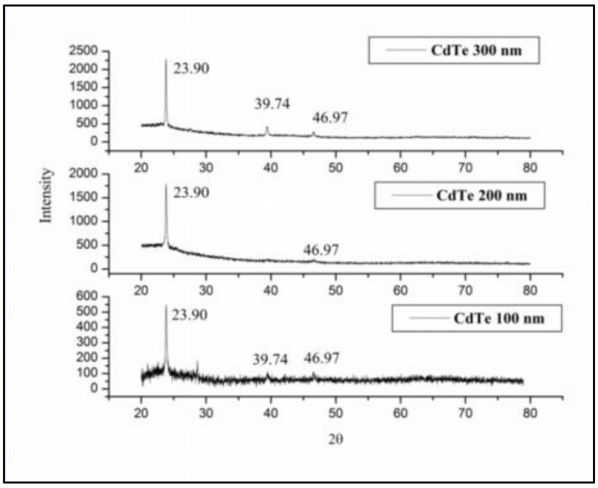

Fig 1: XRD spectra of post deposition annealed CdTe film

Raman Spectroscopy Analysis

Fig. 2 shows first-order Raman spectra of CdTe thin films of thickness 100 nm, 200 nm and 300 nm annealed at 400C. There are three main Raman active modes observed at ~122.2 cm^{-1} ~142.2 cm^{-1} and 164.04 cm^{-1}.The TO and LO modes of CdTe have been found to occur at 142.2 cm^{-1} and 164.4 cm^{-1} respectively[10,11,12,13].. The feature observed at 142.2 cm^{-1} is corresponds to the LO mode of the CdTe [14] while the peak at 164.04 cm^{-1} is due to TO mode[15]. The peak at 122cm^{-1} is related to the TeO_2 Raman vibrational mode[16]

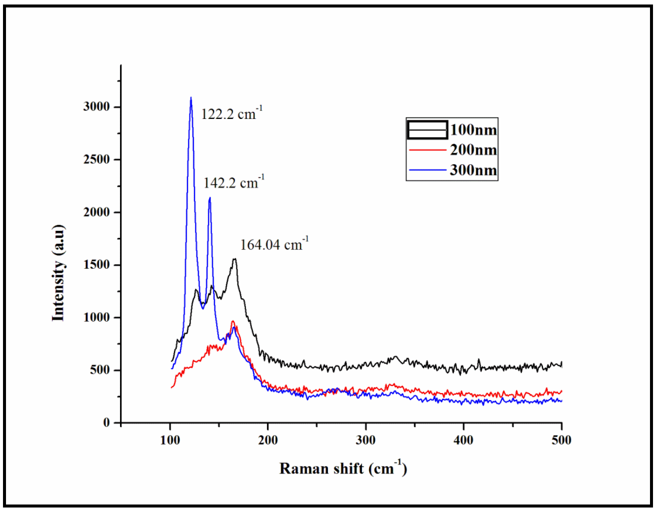

Fig 1: Raman spectra of post deposition annealed CdTe films

EDX Analysis

The compositional analysis for the films of 100 nm, 200 nm and 300 nm annealed films is carried out by EDAX technique. Fig 3 shows the EDAX spectrum of the 100 nm, 200 nm and 300 nm film respectively. The spectrum peak reveals the presence of Cd and Te in the film. EDAX study shows that the Cd to Te ratio is nearly 1: 1 for all the films. However there is a bit higher concentration of Te in the films due to which the films become slightly p-type conducting due to formation of Cd vacancies acting as an acceptor center in CdTe lattice[17]

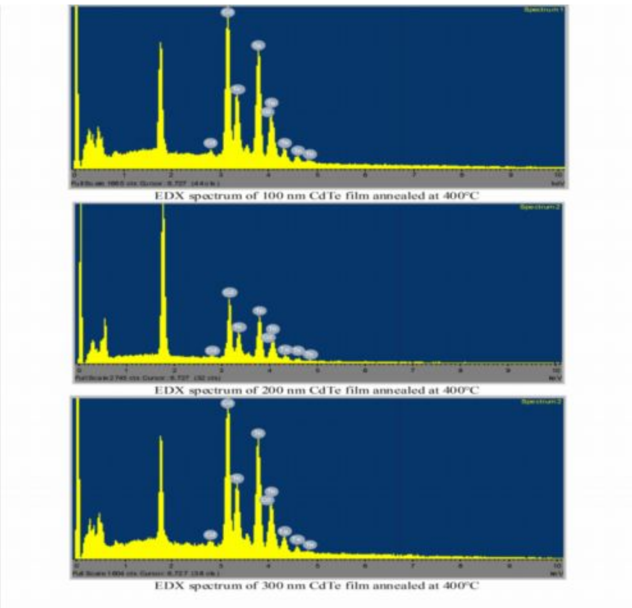

Fig 3: EDX spectra of post deposition annealed CdTe films

Conclusions:

CdTe thin films of different thicknesses are later annealed in argon atmosphere. The phase, structure and composition of the films have been studied. The films are found to be of hexagonal and cubic CdTe structure. The effect of film thickness, annealing temperature on the structural properties depicts increase in the grain size with increasing film thickness. The Raman spectra also reveals peaks corresponding to LO and TO mode of CdTe and the intensity is found to decrease with increasing thickness. The elemental studies shows almost nearly stoichiometric phase of Cdte with slight increase in the Te concentration which could be attributed to the p type nature of the film.

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