J. Fiz. UTM. Vol. 4. (2009) 26-34

X-RAY DIFFRACTION STUDY OF EVAPORATED CADMIUM TELLURIDE THIN FILMS

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ABSTRACT

X-ray diffraction measurement was performed on evaporated CdTe thin films indicating a preferential orientation in (111) direction. The effect of the deposition rate, thickness and substrate temperature was investigated and the film quality was discussed. It was found that as the deposition rate was increased finer crystallite size was obtained, while at the same time the micro-strain decreased. The decrease in crystallite size at higher deposition rate can be interpreted according to the increased velocity and intensity of the vapour atoms during rapid film formation. The crystallite size increased as the substrate temperature was increased up to 200 ^{o}C, above which the crystallite size decreased again. As the thickness was increased the micro-strain decreased, while the crystallite size increased with thickness.

INTRODUCTION

CdTe is an II-VI compound with both p- and n-type character, and it crystallises in both the zincblende and wurtzite structures. CdTe has long been known as an interesting semiconductor with application such as in gamma ray detection [1], electro-optical modulator [2] and solar cell fabrication [3]. Various methods such as evaporation, screen-printing and close-space sublimation have been investigated as suitable techniques for the fabrication of CdTe thin film. Although these processes can prepare CdTe, the resistivity of the films is frequently high. The high resistivity in thin films is partially due to the native defect [2]. Several researchers have investigated the deep levels in n-type CdTe films using space-charge-limited current technique. Basol and Safsudd [4] observed a dominant electron trap located at 0.55 eV below the conduction band with concentration of 10^{15} - 10^{16} cm^{-3} on n-type CdTe films and Gould and Ismail [5] has observed exponential trap on evaporated CdTe thin film. In the present work we describe structural and micro-strain measurement on CdTe thin films.

EXPERIMENTAL

CdTe of 99.99% purity (Balzers) was evaporated from a covered resistively-heated molybdenum boat at a pressure in the range (1.3 to 2.0) x10^{-3} Pa. Corning 7059 substrate was used which could be heated up to approximately 300 ^{o}C during deposition. Substrate temperature was monitored using a thermocouple in direct contact with the substrate. A quartz crystal oscillator placed closed to the substrate monitored film thickness and deposition rate. Thickness was determined accurately after deposition using a Planer Surfometer SF200 stylus instrument. The CdTe films used in this study were deposited at

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rates in the range 0.3 to 1.0 nm s^{-1} with total thickness up to 1 mm. Substrates were maintained at 100, 150, or 200 ^{o}C during deposition.

A Philips X-ray diffractometer (model PW1700), using monochromatic CuK_{α} radiation, was employed to obtain diffraction pattern from film deposited on glass substrates. For this study, continuous scanning was applied with a slow scanning speed and a small time constant. A wide range of 2θ (from 20° to 90°) was scanned, so that all possible diffraction peaks could be detected. XRD line-profile analysis was performed to calculate the crystallite size and residual microstrain, using the technique of Warren and Averbach [6]. Data of the line-profile analysis was obtained using step-scanning technique. An interval of 10 s at each fixed value of 2θ was found sufficient to yield a reasonable number of counts and hence an accurate determination of the peak intensities. A range was selected in which the ordinate returned to the background level before the two ends period. The period was divided into 90 equal intervals ($\Delta(2\theta) = 0.02\,^{o}$) and the number of count during the fixed time interval 91 position was determined. The required calculation were performed using computer software which corrects for the background, the angular variation, the unresolved doublet (using the method of Rachinger), and instrument broadening (using the method of Stoke). A well-annealed quartz sample was used as a strain-free standard sample.

RESULTS AND DISCUSSION

Figure 1 shows the observed diffraction patterns for CdTe films at various deposition rates. In cases the diffraction peak of the [111] plane was very high and the ratio between its height and that of the other peaks was much greater than for randomly orientated films, thus confirming preferential [111] orientation.

Figure 2 shows the particle size and micro-strain as a function of the deposition rate. It was found that as the deposition rate was decreased grain sizes were obtained and at the same time micro-strain increased. The decrease in grain size at higher deposition rates can be interpreted according to the increase of the velocity and intensity of the vapour atoms during rapid film formation, resulting in the formation of more atoms from which fine grains grow. Kawai [7] has observed a similar behaviour in CdTe thin films; films deposited at the lower rate were polycrystalline and those deposited at the higher rates were amorphous. Dislocations as well as other lattice defects may also increase the strain [8]. As the grain size increases the lattice defects decrease leading to a decrease in strain.

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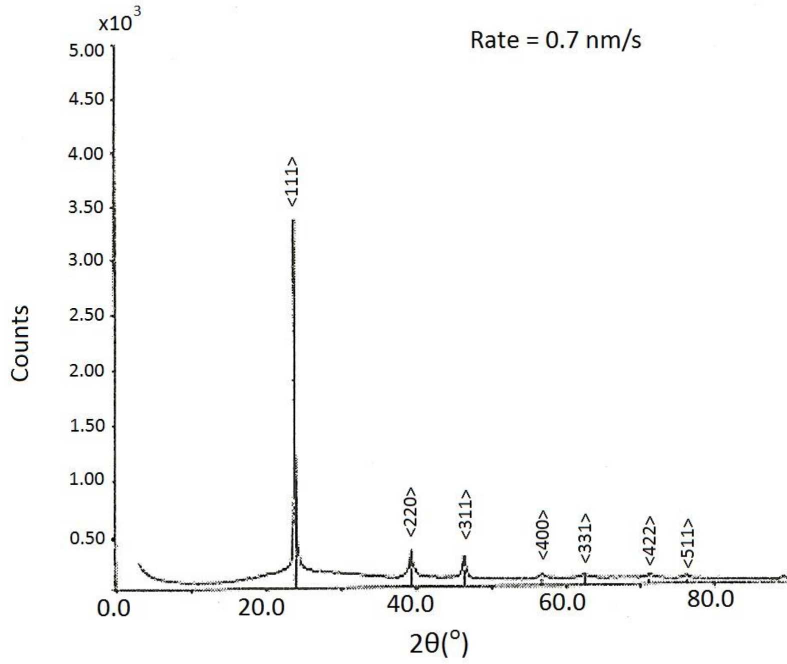
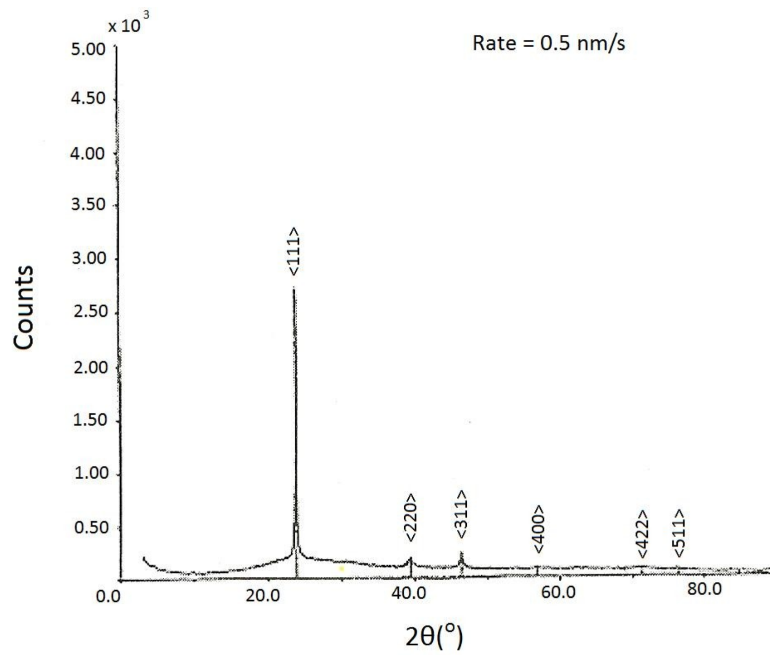


(a) 0.5 nm/s



(b) 0.7 nm/s.

Figure 1: Diffraction patterns of CdTe films for various deposition rates.

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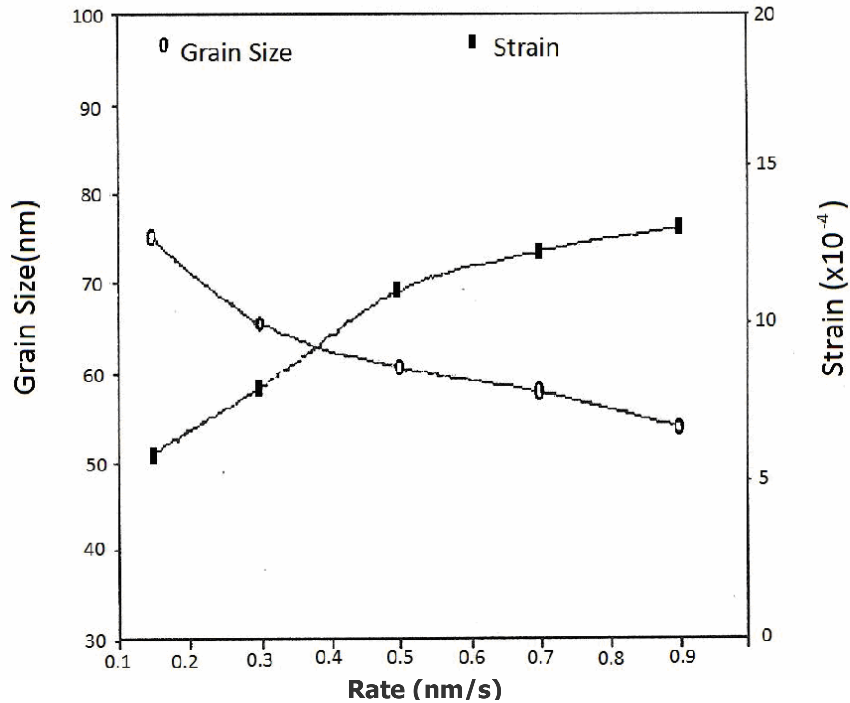

Figure 2: Grain size and microstrain of CdTe films as a function of deposition rate

Figure 3 shows the substrate temperature dependence of the X-ray diffraction patterns of the CdTe films. The diffraction patterns show a clear [111] preferred orientation. In Figure 4, the calculated grain size and micro-strain are shown as a function of the substrate temperature during deposition. These values were derived using slow scans of the [111] peak to obtain data for the computer program. The increase in the grain size as a function of the substrate temperature is probably a consequence of the larger surface mobility of the depositing atoms at higher temperatures, thus there is a decrease in the density of nucleation centres and under these circumstances a smaller number of centres start to grow [9]. The decrease in the size of the crystallites with substrate temperature above 200 ^{o}C is thought to result from the re-evaporation of Cd and Te [10]. The decrease in microstrain with increasing substrate temperature would appear to be related to the larger grain size, as discussed in the previous section.

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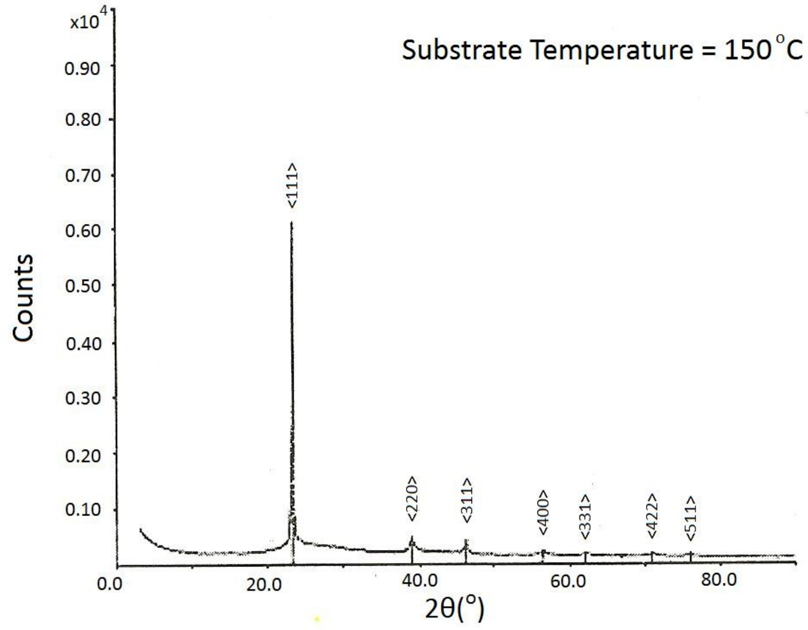
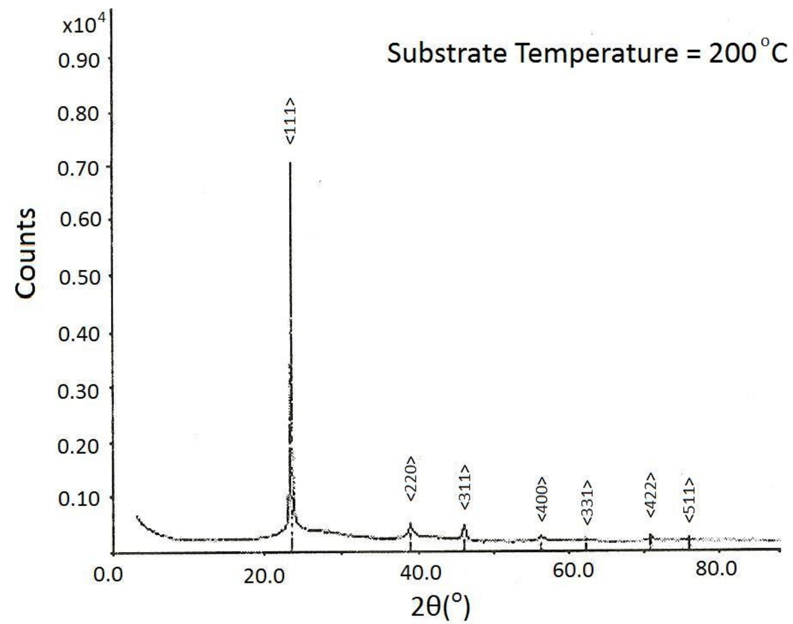


(a) 150 °C



(b) 200 °C

Figure 3: Diffraction patterns of the CdTe films for different substrate temperature.

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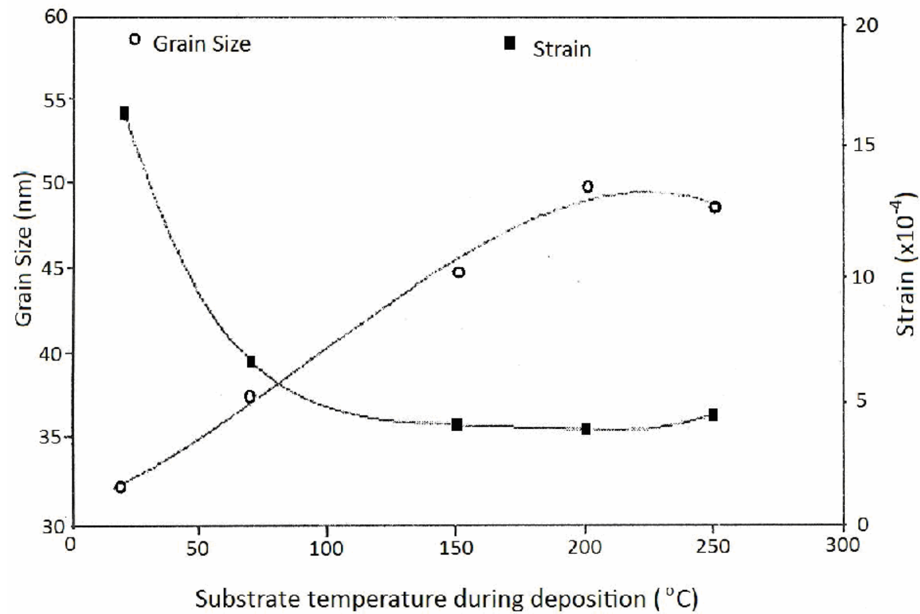

Figure 4: Grain size and microstrain of CdTe films as a function of the substrate temperature.

Figure 5 shows the diffraction patterns for CdTe films at different thickness of 150 nm and 300 nm. The intensity of the [111] X-ray diffraction peak increases with increasing thickness. Figure 6 shows the grain size and micro-strain as a function of the thickness in the thickness range 20 nm - 300 nm, as the film thickness increases, the rms micro-strain decreases while the grain size increases. It is observed that with the increase in thickness of the film there is a gradual increase in the grain size until the film thickness reaches about 70 nm. The grain size tends to have a constant value of about 50 nm for a film thickness above 70 nm. Wilson and Woods [11] have observed similar behaviour on CdS thin films where grain size increases almost exponentially with thickness. Saha et al [12] have observed in CdTe thin films that with an increase in the thickness of the film there is a gradual increase in the grain size and a gradual decrease in the strain and dislocation density for film thickness less than 700 nm. The variation of micro-strain may probably reflect the existence of a strain field around dislocations and has also been observed in the cases of highly deformed metals and alloys [13]

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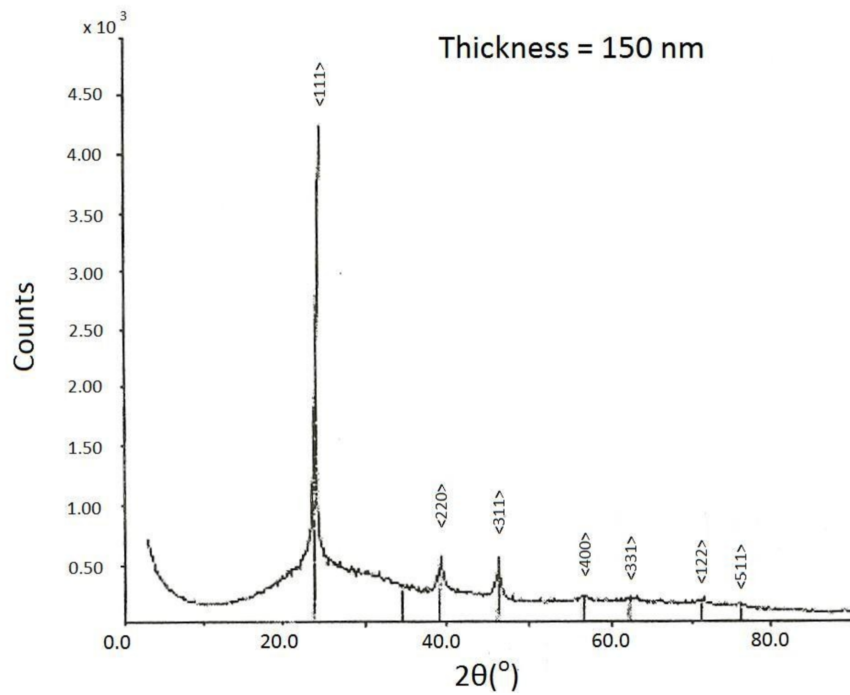
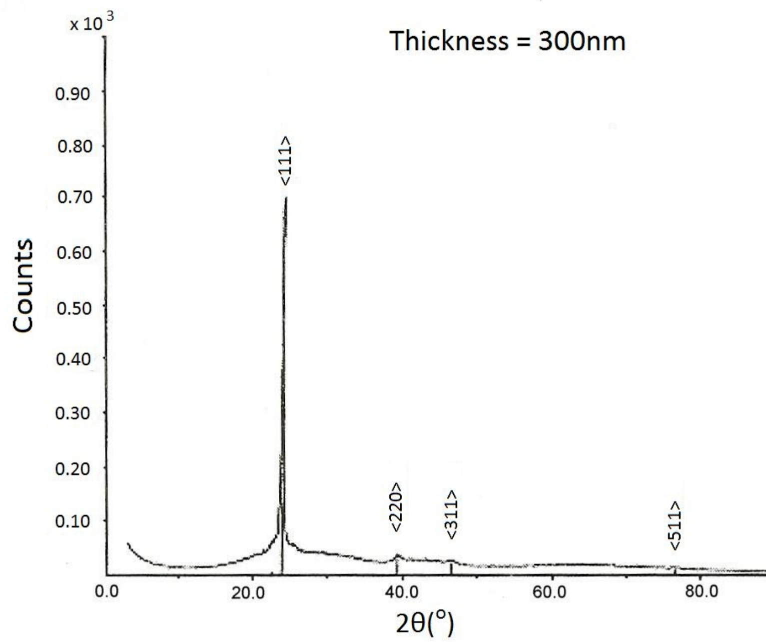


(a) 150 nm



(b) 300 nm

Figure 5: Diffraction patterns for CdTe films for different thickness.

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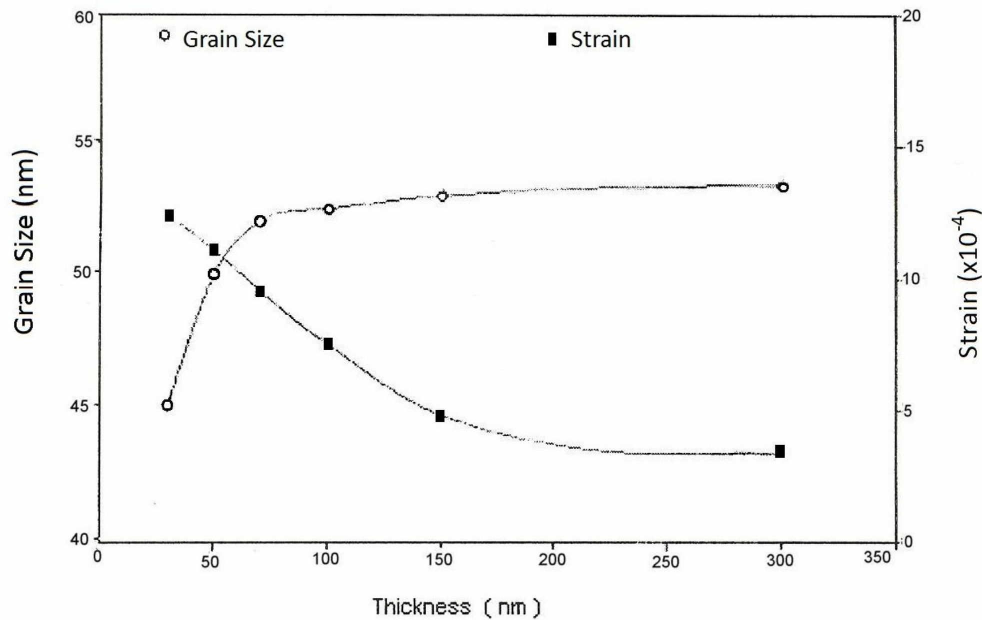

Figure 6: Grain size and microstrain of CdTe films as a function of the thickness

CONCLUSION

X-ray diffraction studies of evaporated CdTe thin films indicate preferential orientation in the [111] direction. The effects of the deposition rate, thickness and substrate temperature on the properties of CdTe films were investigated and the film quality was discussed. It was found that as the deposition rate was increased finer crystallite size was obtained at the same time microstrain decreased. The decrease in crystallite size at higher deposition rate can be interpreted according to the increase of the velocity and intensity of the vapour atom during rapid film formation. The crystallite size increases as the substrate temperature is increased until 200°C, above which the crystallite size decreases again probably due to the re-evaporation of Cd and Te_2 seen take place. As the thickness increase the micro-strain decrease whiles the crystallite size increase almost exponentially with thickness.

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