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STRUCTURAL CHARACTERIZATION OF THIN FILMS OF CADMIUM TELLURIDE*

S. SAHA, U. PAL, B. K. SAMANTARAY AND A. K. CHAUDHURI
Department of Physics and Meteorology, Indian Institute of Technology, Kharagpur 721302 (India)
H. D. BANERJEE
Materials Science Centre, Indian Institute of Technology, Kharagpur 721302 (India)

X-ray diffraction patterns of vacuum-deposited thin films of cadmium telluride have been recorded and X-ray line profile analysis studies have been carried out after correcting for instrumental broadening. Size of the crystallites, r.m.s. strain, dislocation density and stacking fault probabilities have been estimated using the method of variance analysis and peak shift of the line profiles. It is observed that with increase in the thickness of the films there is an increase in the stacking fault probability and this inhibits the growth of the crystallites and results in the increase in r.m.s. strain and dislocation density. The photosensitivity of the films is measured and it is observed, that at about 400 nm thickness, the photosensitivity is at a maximum. An attempt is made to correlate the results.

1. INTRODUCTION

Thin films of cadmium telluride have great potential because of their application as a solar cell material. The influence of the extent of the lattice defects on the photosensitivity of thin films is well known. Kendall[1] has described the peculiarities of the CdTe structure. Semiletov[2] has discussed the dependence of the high voltage photo-e.m.f. in CdTe thin films on the structural properties. Shiojiri and Suito[3] have made a study using electron diffraction of the structure of vacuum-deposited cadmium telluride films and have observed that CdTe films contain a large concentration of stacking faults. However, these works deal with qualitative observation of the defects and grain sizes from electron microscopy. Unlike lead and tin chalcogenides, no quantitative determination of the microstructural parameters such as crystallite size, r.m.s. strain, dislocation density and stacking fault probability has been reported for cadmium telluride. Hence an X-ray line profile analysis study of the different structural parameters in case of semithick (300–1300 nm) films has been undertaken in the present work.

2. EXPERIMENTAL DETAILS

The films are deposited by evaporating CdTe powder from a quartz crucible

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placed in a tungsten coil in a vacuum of the order of 10^{-4} Pa on properly cleaned glass substrates with a Hind Hivac vacuum coating unit (model 12-A4). The rate of deposition is maintained constant at 3.5 nm s^{-1}. The thickness of the films is measured with a surfometer (SF101). X-ray diffraction data are recorded with a Philips X-ray diffractometer using Mo Kα radiation.

The diffracted intensities from the films are of the polycrystalline type and the line profiles were subjected to variance analysis to calculate the crystallite size and microstrain. Since the method is sensitive to the variation near the tails the peaks are carefully corrected for background by the method given by Mitra and Misra[4]. Since the variances are additive the profiles are corrected for instrumental broadening by subtracting the variance of the corresponding profile for standard well-annealed CdTe samples. If it is assumed that the broadening of the X-ray line is due to crystallite size and strain only, the variance can be given by

$$W_{2\theta} = \frac{\lambda\sigma}{2\pi^2 P \cos\theta} + 4\tan^2\theta\langle e^2\rangle$$

where σ is the angular range, P the crystalline size, $\langle e^2\rangle$ the mean square strain, λ the wavelength of the X-rays and θ the Bragg angle. A plot of $W_{2\theta}$ *vs.* σ is a straight line whose slope gives the crystallite size and the intercept gives the strain. Dislocation densities have been calculated from P and $\langle e^2\rangle$ by using the method of Williamson and Smallman[5]. The stacking fault probabilities have been estimated from the peak shift of the X-ray lines by using the method of Warren and Warekois[6]. The plot of variance *vs.* range for the 700 nm film is shown in Fig. 1. The photosensitivity $(\sigma_L - \sigma_D)/\sigma_D$ is measured by using a conventional method[7]. A tungsten filament lamp is used as the source of light and the intensity of the light falling on the sample determined with the help of an Eppley thermopile is maintained constant at 2000 W m^{-2} in all cases. The films deposited in vacuum and exposed to the atmosphere after deposition are found to be p type as determined by thermoelectric measurements.

3. RESULTS AND DISCUSSION

The X-ray diffraction patterns show that the CdTe films deposited on glass substrates are polycrystalline in nature and have an f.c.c. structure with $a = 0.6481$ nm. The crystallites are found to be preferentially oriented with the (111) face parallel to the substrate. The values of the crystallite size, r.m.s. strain, dislocation density and stacking fault probability for films of various thicknesses are shown in Table I. Plot's of stacking fault probability α, dislocation density ρ, microstrain $\langle e^2\rangle^{1/2}$, particle size P and photosensitivity with thickness are shown in Figs. 2(a)–2(e) respectively.

It is observed that with the increase in the thickness of the films there is a gradual increase in the crystallite size and a gradual decrease in the r.m.s. strain and dislocation density up to a thickness of 700 nm. Beyond 700 nm there is a fall in the crystallite size. The stacking fault probability increases with the increase in the thickness of the films.

Cadmium telluride has the zinc sulphide type of structure and can have a close-packed cubic or close-packed hexagonal structure. Both forms can be exhibited simultaneously because of the fact that there is very little difference between the two

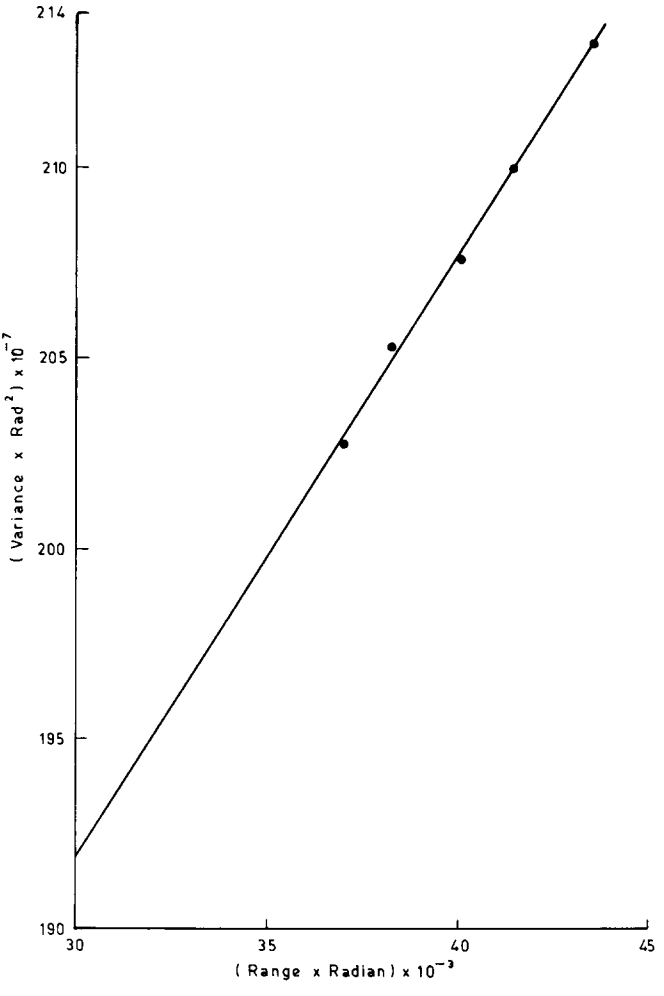

Fig. 1. Variance *vs.* range for the 700 nm film.

TABLE I

MICROSTRUCTURAL PARAMETERS FOR VACUUM-DEPOSITED CdTe THIN FILMS

Film thickness (nm)	*Crystallite size* (nm)	*R.m.s. strain* $\langle e^2 \rangle^{1/2}$	*Dislocation density* (lines m^{-2})	*Stacking fault probability* α	*Photosensitivity at room temperature*
300	4.0	120×10^{-4}	27.772×10^{15}	0.032	0.363
400	7.5	42×10^{-4}	5.5×10^{15}	0.038	1.444
700	20.5	35×10^{-4}	1.6×10^{15}	0.045	0.950
1000	13.0	60×10^{-4}	4.3×10^{15}	0.068	0.270
1300	8.0	82×10^{-4}	9.8×10^{15}	0.130	0.081

structures. The only difference in the zinc blend type (cubic) and wurtzite type of structures is in the stacking sequence of the atomic layers. In the cubic type the stacking pattern of the planes can be represented by ABCABC ... and in the hexagonal type the stacking pattern is represented by ABABAB .... There is very

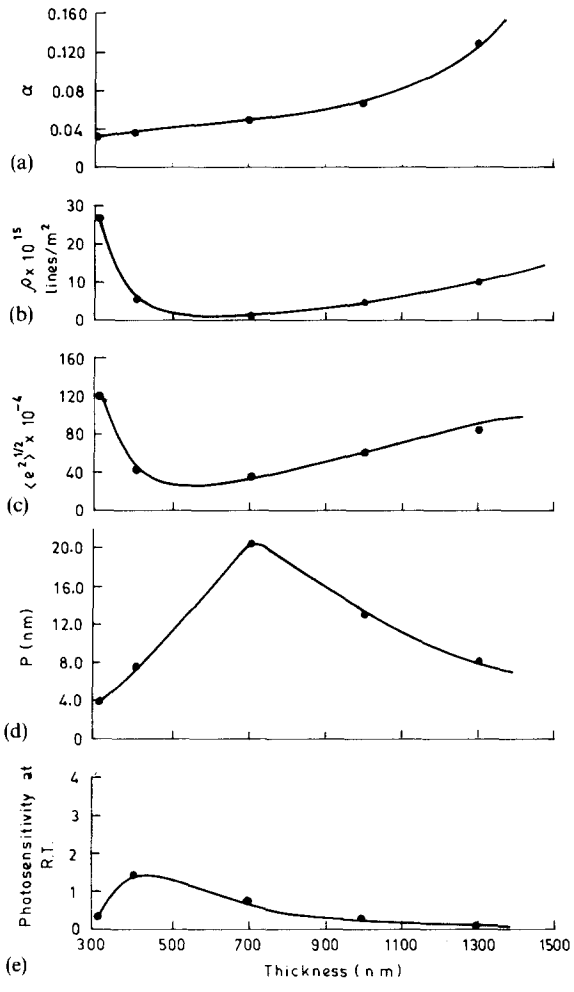

Fig. 2. (a) Stacking fault probability, (b) dislocation density, (c) microstrain, (d) particle size and (e) photosensitivity *vs.* film thickness.

little energy difference between the two types and hence faults in the stacking sequence of one type give rise to the other type in the faulted region. The stacking fault probability α is the proportion of layers undergoing stacking sequence fault and one fault is expected to be found in $1/\alpha$ layers. In the present case the stacking fault probability gradually increases with thickness initially and suddenly increases to a large value for the thick films. Possibly a large concentration of stacking faults for the thick films give rise to the formation of microcrystallites of the other phase and inhibits the growth of the crystallites of the former phase. Probably for this reason there is an initial increase in the size of the crystallites whereas a fall in the size for films of larger thickness is observed.

From the thickness variation of the sensitivity it is seen that the photosensitivity increases up to a thickness of about 400 nm and it starts falling for thicker films. No particular correlation has been observed between the structural parameters and the photosensitivity of the films, which supports the idea that the sensitivity is mainly

related to the formation of a grain boundary potential barrier as a result of diffusion of oxygen at the grain boundary. The maximum value of the grain boundary potential depends on the size and the shape of the crystallites[8], which is found to be at a maximum here at a thickness of 400 nm. However, a faster decrease in the sensitivity of the film is observed when the thickness of the film is greater than 700 nm, which may be due to a sudden increase of stacking fault probability which in turn decreases the size of the crystallites of the film.

REFERENCES

1 E. J. M. Kendall, *Phys. Lett., 8* (1964) 237.
2 S. A. Semiletov, *Sov. Phys. Solid State, 4* (1962) 909.
3 M. Shiojin and E. Suito, *Jpn. J. App. Phys., 3* (1964) 314.
4 G. B. Mitra and N. K. Misra, *Br. J. Appl. Phys., 17* (1966) 1319.
5 G. B. Williamson and R. C. Smallman, *Philos. Mag., 1* (1956) 34.
6 B. E. Warren and E. P. Warekois, *Acta Metall., 3* (1955) 473.
7 N. L. P. Sinha, B. K. Samantaray, A. K. Chaudhuri and H. N. Bose, *J. Phys. D, 9* (1976) 795.
8 J. Y. W. Seto, *J. Appl. Phys., 46* (1976) 5247.