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Structure and properties of vacuum deposited cadmium telluride thin films

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Systematic and detailed study of the growth and properties of vacuum deposited cadmium telluride thin films was made. Both *p*- and *n*-type films were grown and these films were characterized for their structural, optical, and electrical properties. The crystallographic structure of the deposits was found to be dependent on the rate of deposition. Low deposition rates were observed to result in hexagonal deposits whereas high rates of deposition favoured cubic structure for the film. Electrical and optical properties were also found to be dependent on the deposition parameters.

Keywords: Thin films, Cadmium telluride thin films, Cubic structure

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1 Introduction

In recent years, much attention has been shown in semiconducting II-VI compounds because of their opto-electronic properties and their possible applications in switching and memory devices, photodiodes and solar cells. The evaluation of any material for applications is complete and meaningful only when its structure and composition are precisely known. The reliability factor, which is the most important one for device applications, can only be assured through a systematic and detailed study of the structural, electrical and optical properties of the grown films. Hence, due importance has been given to these studies. Cadmium telluride is unique among II–VI series of semiconducting compounds as it shows both *n*- and *p*-type conductivity[1]. Various methods have been used to prepare cadmium telluride thin films[2-6]. But the structure and properties of as obtained films are very sensitive to the deposition conditions. The effect of deposition conditions on the structural characteristics of cadmium telluride thin films has been studied by several researchers[7-12]. The present paper reports an observation of a phase modification resulting from a change in the rate of deposition of cadmium telluride thin films and deposition parameter dependence of electrical and optical properties.

2 Experimental Details

Cadmium telluride thin films were prepared by thermal evaporation of a stoichiometric powder of the compound (chemical purity 99.999% from M/s Research Organic/Inorganic chemical corporation USA) in a residual air pressure of 10^{-5} torr. Molybdenum boat sources were used for the evaporation. Freshly cleaved sodium chloride single crystals, pre-heated to the required temperature served as substrates for structural studies whereas glass slides were used as substrates for optical and electrical characterization. The thickness of the films used for structural characterization was of the order of 50 to 80 nm and that of the films used for electrical and optical characterization was in the range 250–300nm. The grain size was in the range 300-350Å. The structural observations were made on an electron microscope, Philips EM-400, operating at 100 kV in the transmission mode. The compositional information was obtained by EDAX system attached to it.

The electrical characterization involved the study of the variation of resistivity with temperature. Keithley 614 Electrometer has been used for electrical characterization. Thermal activation energies for the conduction have been calculated. Current – voltage characteristics have been studied using different metals as contact materials to obtain a truly ohmic contact material for both *p*- and *n*-type cadmium telluride. Also the effect of post deposition annealing on resistivity has been studied. The carrier type has been determined by conventional hot-probe technique. The optical properties of these films were studied with Shimadzu UV-365 spectrophotometer in the photon energy range 0.5-2.5 eV. The optical band

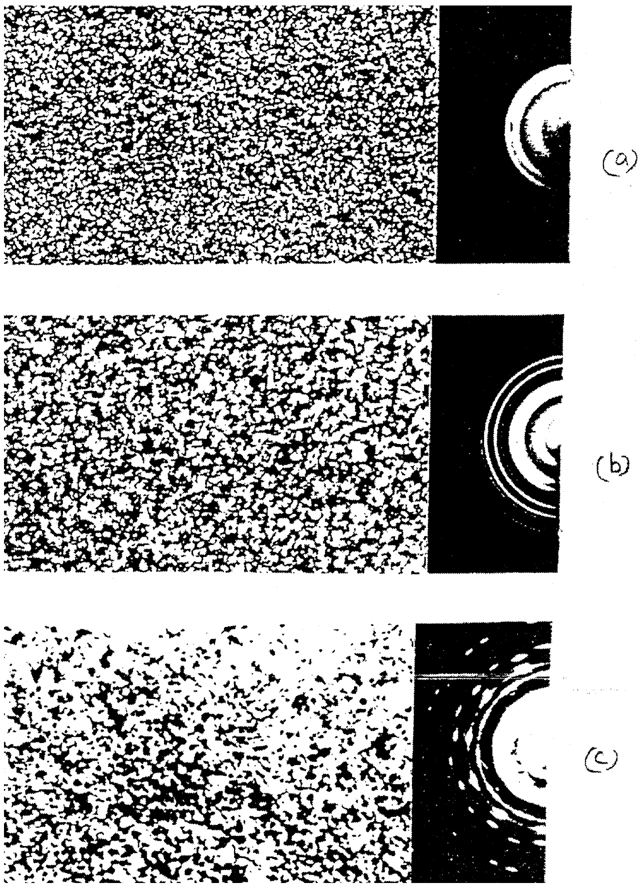

Fig. 1 — Electron micrograph and selected area electron diffraction patterns of CdTe thin films deposited at a rate of 5 nm min^{-1}. Substrate temperatures are (a) 300 K, (b) 375 K and (c) 450 K

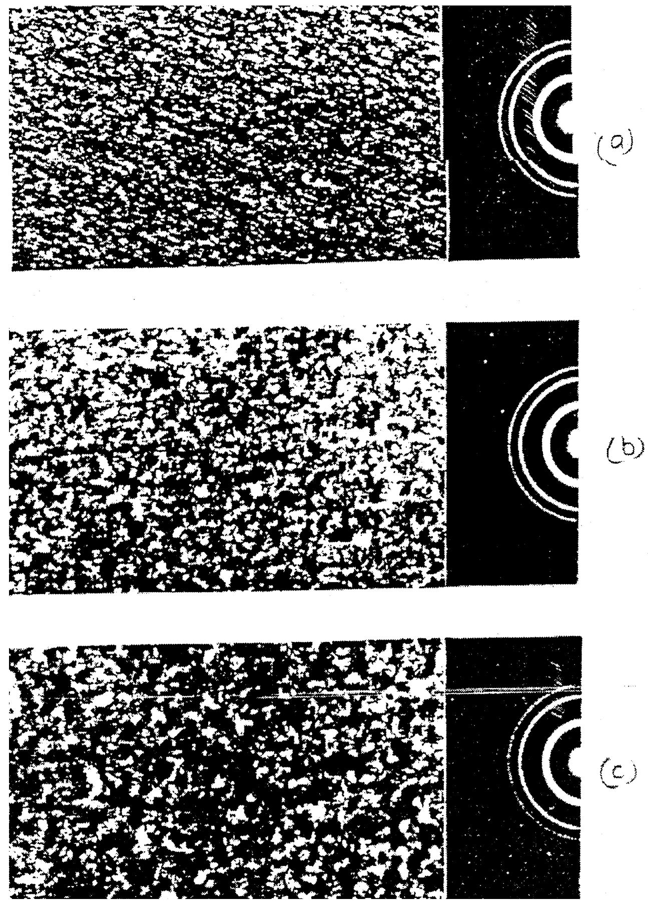

Fig. 2 — Electron micrograph and selected area electron diffraction patterns of CdTe thin films deposited at a rate of 30 nm min^{-1} — Substrate temperatures are (a) 300 K, (b) 375 K and (c) 450 K

gap was found out by optical absorption measurements.

3 Results and Discussion

In the structural characterization of the films, a detailed study of the effect of various growth conditions on crystallinity, chemical composition and phase homogeneity has been carried out. It has been observed that the rate of deposition had a profound influence on the crystallographic structure of the grown films whereas the deposition temperature and post deposition annealing affected electrical and optical characteristics considerably. The deposition was carried out at different rates onto substrates heated to and maintained at different temperatures. Fig.1 shows the electron micrographs and corresponding selected area electron diffraction patterns for films deposited at a rate of 5 nm/min on substrates maintained at various temperatures. The films are essentially polycrystalline in nature and the interplanar spacings computed from the electron diffraction patterns match well with those reported for the hexagonal modification of cadmium telluride (Table 1). Fig. 2 shows the effect of substrate temperature on the structure of films deposited at a rate of 30 nm/min. The films have a cubic sphalerite structure (Table 2). The films deposited at temperature above 473 K showed additional lines in their diffraction pattern, which were identified to be due to the hexagonal phase of the compound. The films obtained at higher substrate temperatures showed a mixture of cubic and hexagonal phases of the compound.

The phase changes without any change in composition are often observed in thin films of chalcogenides[13,14]. Such phase modifications have been reported to depend on deposition

Table 1 — Diffraction data for telluride films (hexagonal) deposited at the rate of 5 nm/min

Observed *d* spacings (nm)	Standard *d* spacings (nm)	*hkl*
0.398	0.3980	100
0.352	0.3520	101
0.227	0.2295	110
0.208	0 2115	103
0.197	0.1995	112
0.170	0.1720	104

*Standard data from ASTM data card no. 19-193

Table 2 — Diffraction data for cadmium telluride films (cubic) deposited at the rate of 30 nm/min

Observed *d* spacings (nm)	Standard *d* spacings (nm)	*hkl*
0.374	0.3742	111
0.230	0.2290	220
0.196	0.1954	311
0.186	0.1871	222
0.162	0.1619	400

* Standard data from ASTM data card no. 15-770.

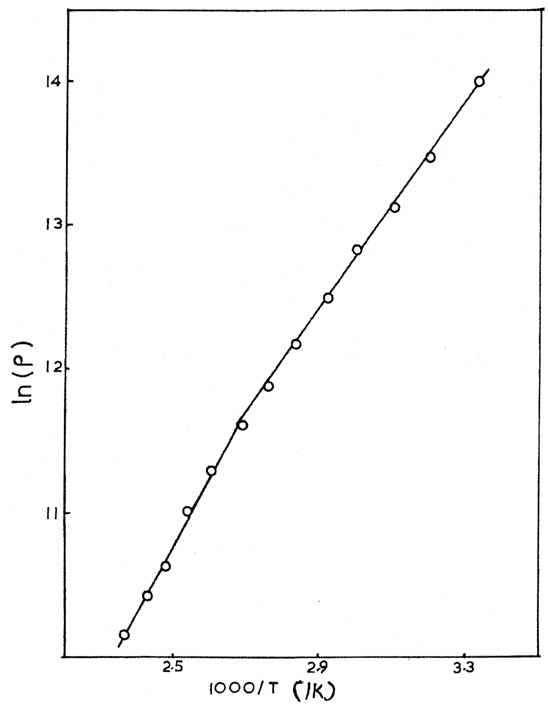

Fig. 3 — Plot of ln*R* versus (1000/*T*) for *n*-type CdTe film deposited at 423 K

temperature[15-17]. Pandey *et al.*[18] have reported growth of cubic and hexagonal cadmium telluride films by pulsed laser deposition. They have observed cubic phase at all pulse energies up to 200 mJ and hexagonal phase at 200 mJ laser energy. The energy difference between the zinc blende structure and wurtzite structure for chalcogenides is very small. It may be inferred that a low concentration of vapour atoms arriving at the substrate, corresponding to a situation obtained at low deposition rates or high substrate temperature, is favourable for the formation of the hexagonal phase.

Post deposition heat treatment has been carried out to study the effect of vacuum annealing on the properties of the films. It may be mentioned that annealing of the films for a period of 5 hr up to a maximum temperature of 523 K did not make any considerable change in the structural properties of the films, except that a marginal increase in grain size was observed.

All the films deposited at room temperature were *p*-type and with a tellurium excess. An analysis of the composition of the films deposited at 300 K by energy dispersive analysis of X-rays revealed the presence of 48.1 and 51.9 atomic per cent of cadmium and tellurium in the films, respectively. Films deposited at 423K were found to be stoichiometric and showed *n*-type conductivity.

Polycrystalline films of cadmium telluride do have the electrical and optical properties similar to those of single crystal films. At the same time, the deposition conditions have been found to have significant effect on the electrical properties[5,6,11,12]. All the films deposited at room temperature were found to be of *p*-type with a resistivity of the order of $\sim 10^7$ Ω cm. Annealing the film at 523K decreased film resistivity by several orders. It may be due to reduction of defects in the films, which act as carrier traps. Also the increase in grain size reduces the resistivity[19]. The band gap energy computed from a study of variation of electrical resistivity with temperature yielded a value of 1.58 eV for these films (Fig. 3). The films deposited at 423 K were found to be of *n*-type with resistivity of $\sim 10^5$ Ω cm. For the *n*-type films, the thermal activation energy for extrinsic and intrinsic regions were found to be 0.65 and 0.74 eV, respectively. The optical absorption coefficient α was calculated from the absorption data near the fundamental absorption edge. An analysis of the spectrum showed that the absorption at the fundamental edge can be described by the relation:

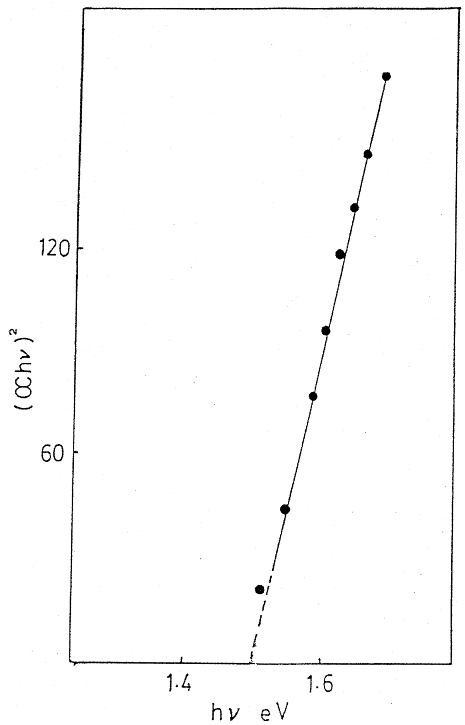

Fig. 4 — Plot of $(\alpha h\nu)^2$ versus $h\nu$ for CdTe film deposited at 423 K showing a direct allowed transition near fundamental absorption edge

$$(\alpha h\nu) = B(h\nu - E_g)^{1/2}$$

where B is a parameter that depends on the transition probability and E_g is the characteristic energy of transition that indicates an allowed direct transition. The energy of transition E_g is calculated from the plot $(\alpha h\nu)^2$ versus $h\nu$ for films deposited at room temperature and at 423K. For room temperature deposited films, the band gap was found to be 1.58 eV (Fig. 4). A small increase in the energy band gap is attributed to the fine grain structure of the as-deposited films. As the substrate temperature was increased to 423 K, the band gap[12,20,21] decreased to the bulk value 1.48 eV.

4 Conclusion

Cadmium telluride films crystallize in two different crystallographic forms, sphalerite and wurtzite structure depending upon the rate of deposition. The lower deposition rates favour wurtzite structure whereas higher rates of deposition result in sphalerite deposits. However, an increase in the substrate temperature favours the wurtzite phase for the deposits. The optical absorption measurements show that the main transition at the fundamental absorption edge is a direct allowed transition with a characteristic energy of 1.48eV.

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