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Growth and characterization of vacuum deposited cadmium telluride thin films

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Semiconducting thin films of cadmium telluride, both *p*-type and *n*-type, have been prepared by conventional thermal evaporation technique. The influence of various growth parameters such as the rate of deposition, deposition temperature, post-deposition heat treatment, and source material composition has been investigated. The films deposited at high deposition rates and low substrate temperatures exhibited an excess of tellurium and showed a *p*-type conductivity, whereas those deposited at high substrate temperature and low deposition rates contained excess cadmium and are *n*-type in nature. An intrinsic bandgap of 1.49 eV for stoichiometric films obtained by both electrical and optical characterization is reported.

II-VI semiconductor compounds are of considerable interest because of their extensive use in the fabrication photo-voltaic devices, photoconductors, IR detectors and solar cells[1,2]. The recent progress in blue-green laser diodes and light emitting diodes with wide band gap II-VI semiconductor[3,4] has attracted much attention for the development of future optoelectronics. Cadmium telluride is an attractive material for photo-voltaic energy conversion having a direct bandgap of 1.58 eV 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 semi-conducting compounds as it exhibits both *n*-type and *p*-type conductivity[5]. Cadmium telluride thin films are attractive materials for the fabrication of semiconductor thin film devices such as γ and IR detectors and field effect transistors[6]. A variety of methods have been used to prepare cadmium telluride thin films[7-11]. But the structure and properties of as-obtained films are very sensitive to the deposition conditions. The influence of deposition conditions on the structural characteristics of cadmium telluride thin films has been studied by several investigators[12-15].

The present paper reports detailed studies carried out on the structural and compositional analysis of cadmium telluride thin films. Detailed analysis has been carried out to identify the nature of absorption edge and to evaluate the characteristic energy of transition. The effect of substrate temperature on the fundamental absorption edge has been analysed. The results of structural, optical and electrical characterization of cadmium telluride thin films are discussed in this paper.

Experimental Procedure

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. Films were also grown by using 2 at.% excess of tellurium with stoichiometric charge. 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 250-300 nm. The structural observations were made on a transmission electron microscope, Philips EM-400, operating at 100 kV. The compositional information was obtained by EDAX system attached to it.

The electrical characterization involved the study of the variation of resistivity with temperature.

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Thermal activation energies for the conduction have been calculated. Current-voltage characteristics were studied using different elements as contact materials to obtain a truly ohmic contact material for both *p*-type and *n*-type cadmium telluride. The carrier type has been determined by conventional hot-probe technique. Optical properties of these films were studied with Shimadzu UV-365 spectrophotometer in the photon energy range 0.5-2.5 eV. Optical band gap was found out by optical absorption measurements.

Results and Discussion

Cadmium telluride thin films were grown under well-defined growth conditions to study their effect on the electrical and optical properties. The major parameters included for detailed study are deposition rate, deposition temperature, post-deposition annealing and the composition of charge material. It has been observed that low rates of deposition less than 5 nm min^{-1}, results in deposits which are having a hexagonal structure (Table 1). An increase in the substrate temperature from 300 to 473 K results in a marginal increase crystallinity of the deposits (Fig. 1). Further, annealing of films up to a temperature of 523 K for a period of 5 h does not produce major changes in either the crystallite size or the crystallinity of the deposits, which remain largely polycrystalline in nature. However, when deposited at a rate of 30 nm min^{-1}, the deposits have exclusively cubic sphalerite structure (Table 2). An increase in the deposition temperature does not produce remarkable change in the crystallinity of the film (Fig. 2).

Table 1— Diffraction data for hexagonal CdTe films. [Fig. 1(c)]

Observed *d*-spacing	Standard *d*-spacing*	hkl
3.98	3.980	100
3.52	3.520	101
2.27	2.295	110
2.08	2.115	103
1.97	1.995	112
1.70	1.720	104

* ASTM data Card No. 19-193

Table 2—Diffraction data for cubic CdTe films [Fig. 2(c)]

Observed *d*-spacing	Standard *d*-spacing*	hkl
3.74	3.742	111
2.30	2.290	220
1.96	1.954	311
1.86	1.871	222
1.62	1.619	400
1.49	1.488	331

* ASTM data card No. 15-770.

The chemical composition of the films deposited under different conditions was also studied in detail. The starting material was a fine powder of stoichiometric compound. All the films deposited at room temperature contained excess tellurium and showed *p*-type conductivity. It is observed that the tellurium content decreases as the deposition temperature increases. The films were stoichiometric at a deposition temperature of 423 K. They exhibited *n*-type conductivity. Further increase in the substrate temperature resulted in the decomposition of the compound with electron diffraction patterns revealing additional lines due to free elements.

The electrical resistivity of the as-grown films was very high and of the order of 10^7 ohm-cm for room temperature deposits which reduced to 10^5 ohm-cm for films deposited at 423 K. The films were also grown using a charge containing 2 at. % excess of

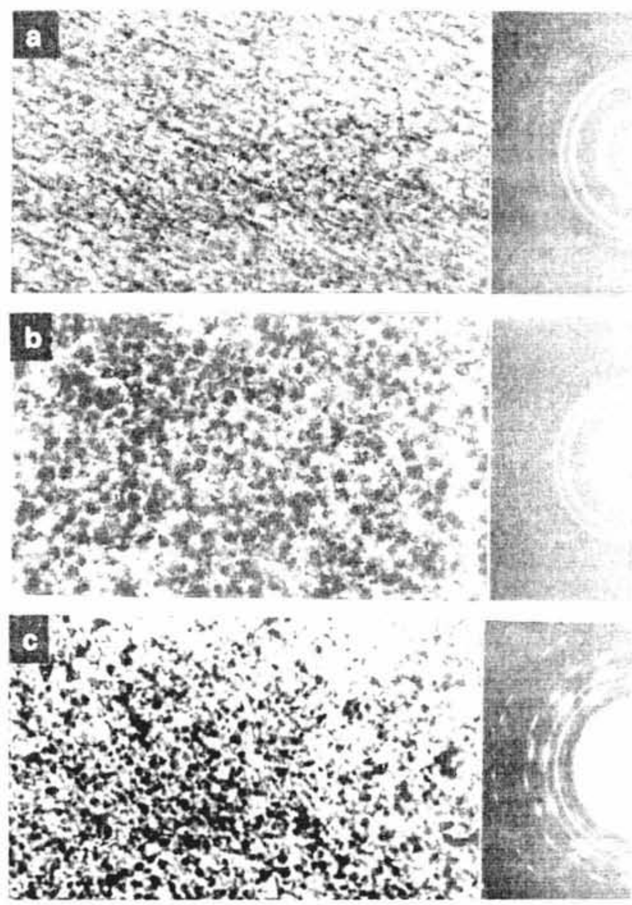

Fig. 1—Electron micrographs (×42,000) and selected area electron diffraction pattens of CdTe thin films deposited at a lower rate of 5 nm min^{-1}, at different substrate temperatures (a) 300 K, (b) 375 K, (c) 450 K

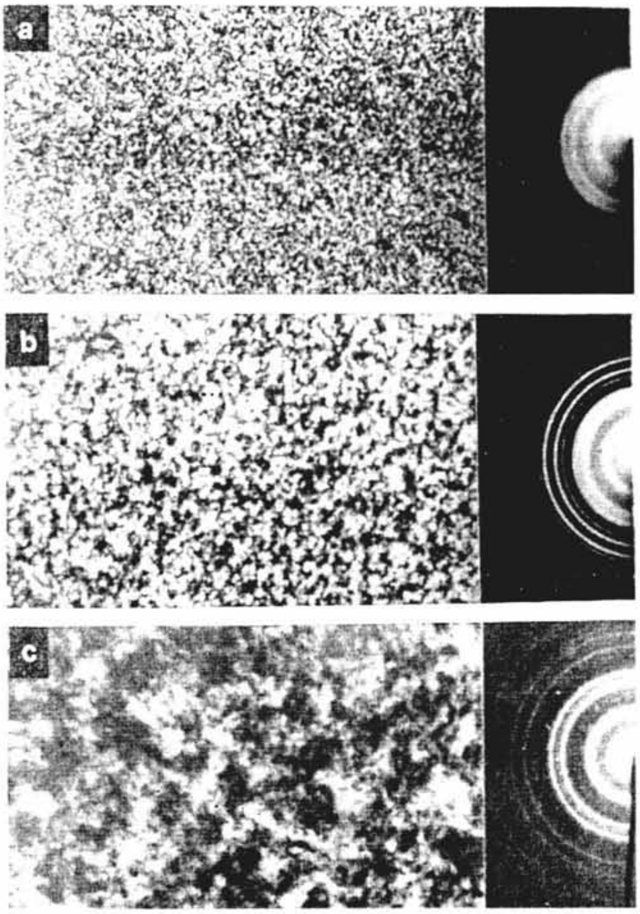

Fig. 2 — Electron micrograph (× 42,000) and selected area electron diffraction patterns of CdTe thin films deposited at higher deposition rate of 30 nm min^{-1} showing cubic Sphalerite structure, deposited at different substrate temperatures (a) 300 K, (b) 375 K, (c) 450 K.

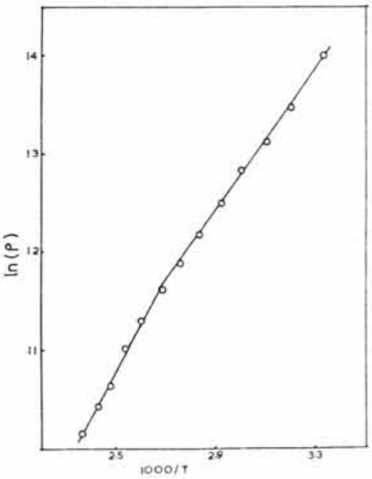

Fig. 3 — Plot of ln(ρ) versus (1000/*T*) for *n*-type CdTe films deposited at 423 K.

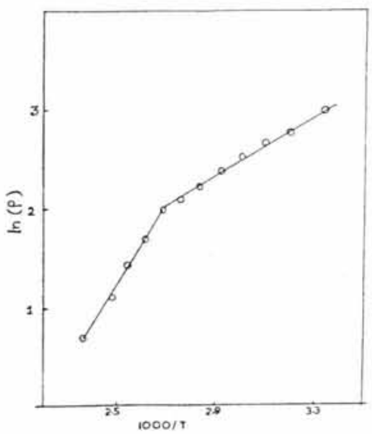

Fig. 4 — Plot of ln(ρ) versus (1000/*T*) for *p*-type low resistivity CdTe films deposited at 473 K.

Table 3 — Experimental data for cadmium telluride thin films

Charge material	Substrate temperature, K	Composition of films	Conduction type	Thermal activation energy, eV		Resistivity, Ω-cm	Optical band gap, eV
				Intrinsic	Extrinsic		
CdTe	423	Stoichiometric	*n*-type	0.74	0.65	10^5	1.49
CdTe+2%Te	473	Stoichiometric	*p*-type	0.75	0.25	$10\text{-}10^2$	1.49

tellurium as the source material. The films grown were stoichiometric at a deposition temperature of 473 K. The films show *p*-type conductivity with resistivity of the order of 10^1 to 10^2 Ω-cm. The fact that they had a composition equivalent to that of a stoichiometric compound but still exhibited *p*-type conductivity indicate that the films may not be homogeneous and may contain free elements contributing to conductivity.

A detailed study of electrode materials for cadmium telluride reveals that indium and cadmium make ohmic contacts to *n*-type cadmium telluride whereas tellurium makes an ohmic contact with *p*-type cadmium telluride. In order to evaluate the activation energy for conduction in these films, the variation of resistivity with temperature was studied in the temperature range 300-473 K (Figs 3 and 4). The results are summarized in the Table 3.

For the films deposited at 423 K, the thermal activation energy near room temperature is found to be 0.65 eV, determined from the slope of the ln(ρ) versus 1000/*T* plot (Fig. 3). This is attributed to the characteristic activation energy associated with the conduction process across grain boundaries[16]. Near stoichiometric films grown using starting material with 2 at.% excess tellurium deposited at 473 K yielded an extrinsic activation energy of 0.25 eV along with an intrinsic value of 0.75 eV.(Fig. 4).

Optical absorption measurements were carried out on films deposited under various growth conditions to evaluate the effect of deposition parameters on the nature of the forbidden energy gap. The study indicated an allowed direct band gap for all the films and the energy of transition calculated for different cases are reported in the Table 3. As-deposited, room temperature deposits were found to have an absorption edge at 1.58 eV whereas film deposited at substrate temperature of 423 K showed an absorption edge at 1.49 eV. The low resistivity film deposited from a charge containing 2 at.% excess tellurium at a substrate temperature or 473 K also showed an allowed direct band gap with an energy of 1.49 eV.

Conclusions

Cadmium telluride films crystallize in two different crystallographic forms, cubic sphalerite and hexagonal wurtzite depending upon the rate of deposition. Post-deposition heat treatment does not produce improvement in the structure as well as the properties of the films. Electrical conductivity measurements suggest an intrinsic band gap of 1.48 eV for cadmium telluride films. The optical absorption measurements show that the main transition at the fundamental absorption edge is a direct allowed transition with a characteristic energy of 1.49 eV. Near-stoichiometric films with *p*-type conductivity and low resistivity can be prepared.

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