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Characterization of Vacuum Evaporated CdTe thin films by XRD, Optical Transmittance and Energy Dispersive Analysis of X-rays

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Abstract: Thin films of thickness 500 nm were deposited by thermal evaporation in a pressure of 5×10^{-5} torr by controlled rate of vacuum evaporation 20 Å/Sec. The as-grown thin films were characterized by X-ray diffraction for structural studies, Transmittance studies were used to for band gap measurements. The band gap was found to be Eg$\approx$ 1.45 eV, The EDAX studies for compositional analysis showed near stoichiometric ratio and Williamson-Hall studies for the crystallite size & microstrain determination were performed using the XRD data. The thin films showed an average crystallite size $\approx$ 75 nm. The variation of refractive index with wavelength was studied. The plot was linear and showed a decrease in refractive index with increase of wavelength (λ).

1. Introduction

Semiconductors of the Chalcogenide type have been a source of attraction in recent times due to their band gap in the visible region. Alloys of Chalcogenide type like CdTe have been studied in the bulk form and in thin film form. There have been many techniques through which thin films have been grown. However CdTe thin films deposited by thermal vacuum evaporation have been done by a few researchers [1-2]. The technique of thermal evaporation has an added advantage due to the fact that thickness of thin films of CdSe in calculated levels can be obtained by thermal evaporation by precise monitoring with single direction deposition. The physical properties of CdTe thin films have been studied here in our work for the as-grown CdTe thin films.

2. Experimental

Highly pure Cd and Se materials (99.999%) were taken and weighed stoichiometrically in an electronic balance. These alloy materials were kept in an quartz ampoule and the ampoule was sealed in a vacuum of 5×10^{-5} torr. The evacuated ampoule was sealed by glass blow apparatus. The ampoule was vertically hung in a wire wound muffle furnace. The furnace was heated step wise initially to the melting point of Cadmium at 320 °C for

5 hours. The furnace temperature was gradually elevated to the melting point of Tellurium (≈ 450 °C) Initially Cadmium diffuses into Te and then both the melted elements form a homogenous mixture. The furnace temperature is elevated to a higher temperature of 600 °C with constant *in-situ* shaking. The homogenous mixture is cooled step wise and the quartz amopoule is broken with care to isolate the CdTe alloy. This CdTe alloy is cleaned with ethanol and dried. The CdTe alloy is properly grinded to a fine powder form. The alloy powder is kept in a desicator to keep it away from moisture. The properly cleaned glass plates with carbon tetrachloride are dried by air blower to remove surface impurities. The glass plates are kept in a vacuum chamber with an ambient pressure of $\approx 5 \times 10^{-5}$ torr Tantalum boats were used in the vacuum system for the thermal evaporation of CdTe. A.C. current of 15 Amps was used to evaporate the the material at the rate of 20 ± 1 Å/Sec and the growth of the thickness (≈ 5000 Å) of CdTe thin film was monitored by Quartz Crystal monitor. The Powder Diffraction was conducted by using Philips X-ray machine using Cu-K_α as the target X-ray radiation. The sample was scanned with X-rays from 5^o to 80^o to realize all diffracting planes. A Hitachi (Model No. UU 340) UV-VIS-IR spectrophotometer was used to study optical absorption of the semiconductor, CdTe between the wavelengths 400 - 900 nm of for its optical band gap measurement.

3. Results and Discussion

3.1 Structural Characterization of CdTe thin films

The as-grown thin films of CdTe were subjected to powder X-ray diffraction. The XRD pattern was compared with the bulk XRD pattern of the same material. There were many peaks in the bulk. The preferred direction of the growth of the thin film lead to some less peaks in the thin film XRD pattern. The d-values of the bulk and the d-values of the thin films match fairly. The Fig. 1.(a) shows the typical XRD pattern for the CdTe bulk and Fig. 1(b) shows the XRD pattern of CdTe thin films. From the powder XRD pattern it was found that the thin films exhibit Zinc Blende structure with the lattice constant $a_o \approx 6.482$ Å as per the JCPDS Card No. 75-2086 belonging to the space group of $F\bar{4}m$. The lattice constant, a_o is calculated using the formula:

$$\frac{1}{d^2} = \frac{h^2 + k^2 + l^2}{a_o^2}$$

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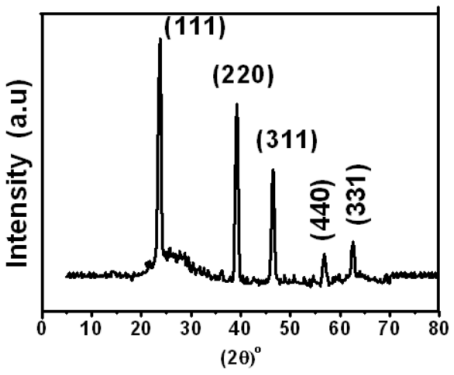

Fig. 1 (a) XRD Pattern of a CdTe Powder

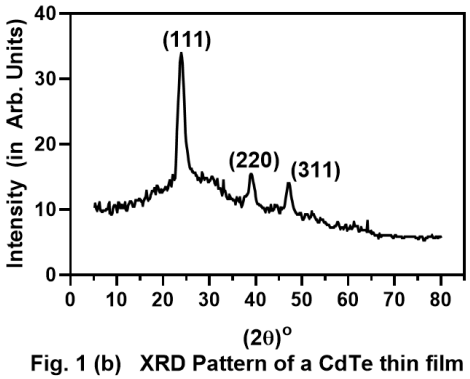

Fig. 1 (b) XRD Pattern of a CdTe thin film

The lattice microstrain (ϵ) was calculated using the XRD pattern for the thin film using the Williamson Hall method [3] by taking the slope of the curve of $\beta cos\theta$ vs $Sin\theta$ (as shown in Fig. 2) The value of (ϵ) was found to be ≈ 0.00185. The crystallite size as calculated from the formula was found to be ≈ 750 nm.

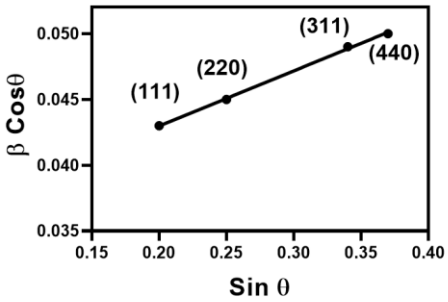

Fig. 2. Crystallite strain separation calculated using line width β according to "Williamson–Hall" method

3.2 Optical Transmittance studies on CdTe thin films

Thin films of CdTe were characterized by optical transmittance studies. The variation of Transmittance vs Wavelength is shown in Fig. 3. It is seen that transmission plot swings for the wavelengths from 900 nm to 1500 nm region in an oscillatory manner. The refractive index (n) is calculated by the method of swings in the transmittance spectra [4]. It is seen that refractive index (n) decreases with the increase in wavelength. Figure 4. shows the variation of refractive index (n) with wavelength (λ) . The band gap was Eg ≈ 1.45 eV from transmittance studies matches well those with literature [5].

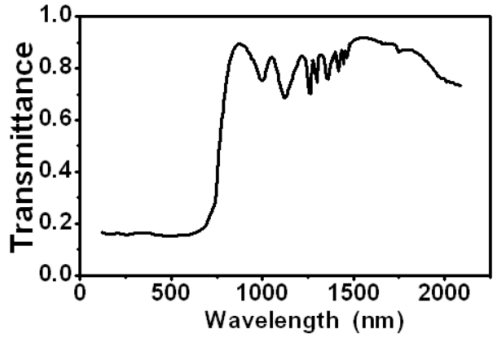

Fig. 3. Transmittance vs Wavelength

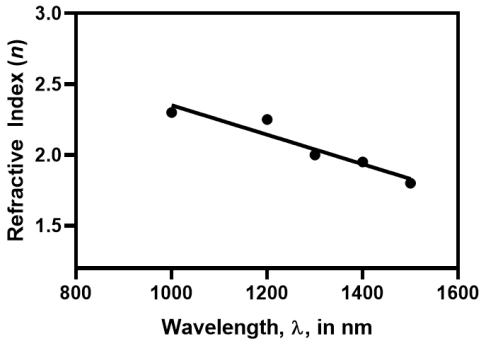

Fig. 4. Variation of Refractive Index (n) with Wavelenght (λ)

3.3 Energy Dispersive Analysis (EDAX) of CdTe thin films

Thin films of CdTe were characterized by EDAX studies for compositional analysis. A typical EDAX spectrum of the as-grown thin film of CdTe is shown in Fig. 5. It is seen that the integrated counts for Cd-L_α, Se- L_α were quantitatively analyzed by MICROZAP software program accompanying the EDAX set up. The integrated intensities of the Cd-L_α and Se-L_α obtained for the thin film material were analyzed by comparing with the intensities of the standard profile. It is found that the atomic composition was for Cd $\approx 49.56 \pm 1.2$ % and for Te $\approx 49.46 \pm 1.3$ %. Which is nearly the same as the starting bulk CdTe alloy.

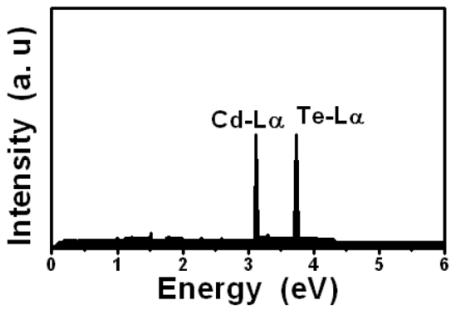

Fig. 5. EDAX Spectrum of a CdTe thin film

4.0 Conclusions

The thin films of semiconducting CdTe were characterized by powder XRD to know its structure. It was found that the thin film exhibits cubic symmetry. The miller indices, viz., *hkl* match with those values given in the literature. The lattice constant calculated by powder XRD diffraction was $a_o \approx 6.482$ Å. The microstrain (ϵ) calculated by Williamson-Hall method (ϵ) was found to be ≈ 0.00185. The variation of refractive index (n) with wavelength (λ) was found to agree with other workers in the literature. The CdTe thin films were characterized for compositional analysis by EDAX and the thin films showed near stoichiometry. The as-grown thin films of CdTe deposited by thermal evaporation had lesser peaks in the powder XRD pattern due to preferential planes in the thin films during the thin film growth/deposition thus supporting X-ray diffraction as per the Bragg's equation. The low value of lattice microstrain suggests that the thin films have potential application for usage in fabrication of devices like thin film solar cells

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