Optical Characterisation of CDTE Thin Films

Desh Bandhu Sharma

Department of Physics, G. G. M. Science College, Jammu, India

Abstract: We report the results obtained from the optical Characterisation of CdTe thin Films grown by Flash Evaporation technique. The objective of this work is to determine its stability for optoelectronics devices. Important aspects in CdTe thin films optimisation of deposition conditions and effects of photo thermal annealing in hydrogen environment on the optical properties are also investigated.

Keywords: Absorption Spectra ; Band Gap ; CdTe ; Flash Evaporation ; Optical Characterisation ; Reflectance Spectra ; Thin Films

1. Introduction

Cadmium Telluride Thin films have a very importance place in the semiconductor industry. They have been investigated extensively for the development and production of Photovoltaic (1, 2) optoelectronic (3) and IR devices (4). In recent years CdTe has emerged as a potential material for HgCdTe photo diodes since its a wide gap semiconductor which is nearly lattice matched and chemically compatible to MCT (5, 6). Some work has been carried out on single crystal of CdTe (7, 8). CdTe Eplayers were grown by MOCVD (9-12), Sputtering (13) and Thermal Evaporation (14-15) and Electron Beam Evaporation (16).Unfortunately the preparation of high quality stoichiometric films is very crucial problem with the material and require stringent growth conditions. To overcome this problem, we deposited thin films by Flash Evaporated Technique. Cadmium Telluride thin films were deposited by Flash Evaporation technique which is very simple and convenient method. Since a very little information was available on deposition of CdTe by this technique, a very careful study was under taken on various parameter involved in the deposition of CdTe thin films. For the deposition of CdTe thin films by Flash Evaporation system, the following growth conditions were optimised and used.

1) Vacuum in chamber ~ $10^{-6}$ torr
2) Deposition temperature ~ Room Temperature
3) Boat temperature ~ 1400°C
4) Deposition Rate ~10Å/ Sec

In the Flash Evaporation technique a proper selection and control of evaporation boat and substrate temperature provide adequate control of stoichiometry of the films. Here a very small quantity of the CdTe material was dropped into the preheated boat, resulting in its instantaneous (Flash) evaporation. It was observed that a lot of material was lost by splattering if a simple open boat was used for Flash Evaporation. In addition to this the deposited films appeared to be uneven with pin holes. This could be possible due to deposition of some very fine splattered grains of source material which got carried on to the substrate by the stream of evaporated material. It was not possible to reduce splattering by increasing the boat temperature. This problem was, however, overcome by employing a modified design of the evaporation boat. This boat was covered by a cover which had an entrance aperture and a large number of exit apertures. Its size was optimised to ensure that the amount of evaporated material fed into the boat through the hole was minimum. This particular design of boat was found to almost prevent splattering and preferential loss of the more volatile components.

2. Experimental Technique

Thin Films of CdTe were deposited on optically polished glass, mica and quartz substrates, under a vacuum of $10^{-6}$ torr. Prior to deposition, the glass microslides, quartz and mica substrates were subjected to extensive cleaning. For this purpose, the substrates were initially thoroughly washed with liquid detergent and later rinsed repeatedly in distilled water. These were boiled in 50% nitric acid solution for fifteen minutes followed by thorough washing with deionised water. The substrate was then degreased in vapours of isopropyl alcohol. The substrates were mounted in the rotating substrate holder which was held in the vacuum chamber such that substrates were located at a distance of ~15cm from the evaporation boat. A molybdenum boat with cover having a 3.5mm diameter entrance aperture for the source material and a large number (25) exit apertures of 0.75mm diameter each was used for evaporation. The boat cover was used to minimize the effects of splattering. The material was intermittently fed by the hopper- vibrator arrangement of the flash evaporation jig, onto the preheated boat. The boat was maintained at ~1400°C. The film growth was continuing till the appropriate thickness was obtained. A quartz crystal monitor was used to control the deposition rate and thickness of the film. The substrate holder was rotated slowly to obtain uniform thick films. The film growth was continued till films with appropriate thickness were obtained. A quartz crystal monitor was used to control the deposition rate and thickness of the film. The starting material was CdTe powder from Balzer’S 99.9% purity.

Optical Characterisation

The Hitachi 330 spectrophotometer was used to obtain the transmittance and reflectance spectra. For the absorption measurements the films were deposited on quartz crystal were used. The effect on the thin films by the absorption of incident radiations in the supporting substrate was eliminated by keeping reference substrate in the path of an incident beam in the spectrophotometer. The slit width employed during transmission and reflectance measurements correspond to those defined for automatic operation of the instruments. Absorption coefficient

Optical transmittance, reflectance and absorbance spectra were measured within the range 185nm-2500nm. The
Hitachi 330 spectrometer was used to obtain the transmittance and reflectance spectra. For the absorption measurement of the thin films deposited on microglass slides were used. Absorption coefficient (α) value at a particular wavelength (λ) was calculated from the experimentally measured transmittance and reflectance (R) values using relation

$$\alpha_\lambda = \frac{1}{d} \ln \left[ \frac{(1-R^2)}{2T} + \frac{(1-R^4)}{4T^2} + R^2 \right]$$

where d is the thickness of the film. Films used for optical absorption measurement were 1500-9000Å. Film thickness was determined by using a Talyor-Hobeon Talystep instrument. It is well known that absorption coefficient for direct transition is of the form

$$\alpha = \begin{cases} a (h\nu - E_g)^{1/2} & \text{for } h\nu > E_g \\ 0 & \text{for } h\nu < E_g \end{cases}$$

In such transition the K vector of the electron remains constant except for very small and entirely negligible change caused by absorption of the photon. Thus for an allowed direct band gap transition, the Absorption coefficient related to photon energy given by

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

Where 'A' is constant and $E_g$ is the energy gap. Therefore for direct band gap semiconductor, $(\alpha h\nu)^2$ Vs $h\nu$ characteristics is expected to be a straight line, with the photo energy axis intercept giving the value of the band gap.

Two sets of CdTe films of thickness ~ 4000Å were deposited on quartz substrates. First set comprises of five samples of CdTe films, prepared after employing the hydrogen annealing at 80°C in pressure of UV photon having wavelengths range between 185nm and 254nm. The annealing was carried out in a photo chemical vapour deposition unit, in which the hydrogen vacuum was maintained at 1mbar. The annealing duration was varied from 0hour to 4hours. During the process hydrogen was directly passed into the chamber.

The second set of four CdTe films was made by varying the hydrogen annealing duration from 0hour to 3hours at 80°C in pressure of UV photons. During this process hydrogen was bubbled through Hg boat maintained at 100°C.

The optical transmittance and reflectance spectra of the films in the range 500nm to 1500nm were recorded using Hitachi 330 UV-VIS-NIR spectrophotometer. Spectral variations of the absorption coefficient $\alpha$ (cm$^{-1}$) in the range 1.2eV to 1.6eV for both sets of CdTe films as shown in Fig. 1 and2. The $\alpha$ value at particular wavelength or energy has been calculated from the experimentally measured transmittance and reflectance values. It is observed from the fig.1 for 1st set of $\alpha$ Vs $h\nu$ plot that the absorption coefficient shifts towards lower wavelength with increase in hydrogen annealing durations at 80°C in presence of UV photon.

![Figure 1: Variation of Absorption Coefficient as a Function of Photon Energy for CdTe films annealed in hydrogen atmosphere at 80°C in presence of UV photon. During the process hydrogen was directly passed into the chamber.](image1)

![Figure 2: Variation of Absorption Coefficient as a Function of Photon Energy for CdTe films annealed in hydrogen atmosphere at 80°C in presence of UV photon. During the process hydrogen was bubbled through Hg- tub maintained at 100°C.](image2)
For 1st set, hydrogen was directly passed into the cham1ber and for 2nd set hydrogen was bubbled through Hg tub was maintained at 100°C. The values of \((\alpha h\nu)^2\) as derived from transmittance and reflectance data has been plotted in Figs. 3 and 4 for both sets as function of photo energy \(h\nu\). The values of optical band gap were determined by extrapolating the linear part of the plot \((\alpha h\nu)^2\) Vs \(h\nu\) to the energy axis. The values of band gap thus obtained for 1st set and 2nd set have been presented in table 1 and 2 respectively.

![Figure 3: \((\alpha h\nu)^2\) as a Function of Photon Energy for CdTe films annealed in hydrogen atmosphere at 80°C in presence of UV photon. During the process hydrogen was bubbled through Hg-tub maintained at 100°C.](image)

<table>
<thead>
<tr>
<th>S.No.</th>
<th>Annealing Duration in Hydrogen without employing Hg tub (Hours)</th>
<th>Band Gap (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0</td>
<td>1.435</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>1.44</td>
</tr>
<tr>
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</tr>
<tr>
<td>4</td>
<td>3</td>
<td>1.46</td>
</tr>
<tr>
<td>5</td>
<td>4</td>
<td>1.495</td>
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</table>

For the CdTe thin films annealed in hydrogen atmosphere at 80°C in presence of UV photons, when hydrogen was directly passed into the chamber during the process, the optical band gap increased with increase in annealing duration as shown in table 1. The increase in band gap with increase in hydrogen annealing duration indicates improvements in the crystallinity of CdTe. On the other hand in the annealing process (80°C in presence of UV photons) when hydrogen was bubbled through the Hg tub maintained at 100°C the CdTe thin films showed a decrease in band gap with in annealing duration from 0hour to 3hours as shown in table 2. The decrease in band gap with increase in hydrogen annealing duration, when hydrogen was passed through a Hg tub maintained at 100°C, could be due to the fact that Hg is incorporated into CdTe thin films and this could disturb the crystal structure of CdTe thin films and this could disturb the crystal structure of CdTe. So that the CdTe films showed a decrease in the optical band gap with increase in annealing duration.

<table>
<thead>
<tr>
<th>S.No.</th>
<th>Annealing Duration in Hydrogen with employing Hg tub (Hours)</th>
<th>Band Gap (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
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<tr>
<td>2</td>
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<td>2</td>
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<td>4</td>
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</table>

3. Conclusion

The CdTe Flash Evaporated thin films after annealing in hydrogen atmosphere at 80°C in presence of UV photons, where hydrogen was directly passed into the chamber shows improvement in the band gap, So the Flash Evaporation CdTe films after annealing in hydrogen at 80°C can be suitable optimum material for optoelectronic devices.

References

Thin films edited By K. L Chopra and T.C. Goyal
(Vanity Books, Delhi, p-210) (1981)
71 P5050 (1992)
(1992)
655(1995)
[12] Y. Nemirovsky, N. Amir et. al., J. Electron, Mater.24,
P647 (1995)
[14] J.P. Hirth and K. L. Moazed, Physics of Thin Films,
Vol.4, Edited by G.Hass and R.E. Thun, (Academic
pres. New York, P-97) (1967)
[15] P. B. Barna, A. Barna et.al. ACTA Physics, Academic
Scientiarum Hungaricae, Tomus 49 (1-3), 77 (1980).
[16] J.L. Pankove And N.M. Johanson, Hydrogen in
Semiconductors and Semimetals edited by J.I PanKove
and N.M. Johanson (Academic Pres, New York Vol-3)
(1991)
[17] D. B. Sharma, P. Kashyap et.al. Physics of