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Optimization of Deposition Conditions and Photothermal Annealing of CdTe Thin Films for HgCdTe Passivation Applications

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Abstract: ***This study investigates the optimization of flash evaporation deposition conditions for CdTe thin films intended for HgCdTe passivation applications. CdTe films were deposited under optimized vacuum, boat temperature, and deposition rate conditions, followed by structural, optical, and electrical characterization. XRD confirmed zinc-blende phase formation, while EDAX indicated near-stoichiometric composition. Photothermal annealing in hydrogen significantly influenced film properties. Direct hydrogen annealing increased room-temperature resistivity from 2.4 × 10^4 ohm-cm to 3.23 × 10^5 ohm-cm and increased optical band gap from 1.435 eV to 1.495 eV with increasing annealing duration. Hydrogen treatment in the presence of mercury reduced resistivity and band gap, indicating altered defect behavior. The findings suggest that optimized CdTe thin films are suitable candidates for HgCdTe passivation in infrared detector applications.***

Keywords: CdTe thin films, flash evaporation, HgCdTe passivation, photothermal annealing, semiconductor thin films, optical band gap, electrical resistivity, infrared detectors

1. Introduction

This investigation is relevant to the development and production of photovoltaic (1-2), optoelectronic (3) and IR (4) devices. In recent years, CdTe has emerged as a potential passivant material for HgCdTe photodiodes since it is a wide gap semiconductor which is nearly lattice matched and chemically compatible with HgCdTe (MCT) (5, 6). It is transparent to IR radiation, non- hygroscopic and mechanically harder than HgCdTe (MCT). Various techniques have been employed for the deposition of CdTe, viz. Sputtering (7-8) MOCVD (9-12), Thermal evaporation (13-15) and Electron beam evaporation, etc. Unfortunately, the preparation of high-quality stoichiometric films is a crucial problem with this material and requires stringent growth conditions. To overcome this problem, we deposited CdTe thin films by the Flash evaporation technique (16). The objective of this work is to determine the suitability of CdTe thin film for passivation of HgCdTe by optimising the deposition conditions and the impact of Photothermal Annealing in a hydrogen environment on the properties.

2. Experimental Procedure

Thin films of CdTe were deposited on optically polished glass microslides, mica substrates and quartz substrates, under a vacuum of ~10^{-6}Torr. Prior to deposition, the glass microslides, mica substrates and quartz substrates were subjected to extensive cleaning. For this purpose, the substrates were first thoroughly washed with liquid detergent and later rinsed repeatedly in distilled water. These were then boiled in 50% nitric acid solution for fifteen minutes followed by thorough washing with deionized water. The substrates were 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 the substrates were located at a distance of ~15cm from the evaporation boat. A molybdenum boat with cover having a 3.5 mm diameter entrance aperture for the source material and a large number (25) of exit apertures of 0.75 mm diameter each was used for evaporation. (Fig.1). The boat cover was used to minimise 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 continued 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 of 99.9% purity. The compositional analysis of the films were carried out using a PV 990 EDAX attachment on a Philips SEM 515 Model. A UV-VIS-IR Hitachi model 330 was employed to record the transmission and reflection spectra in the wavelength range 500-2000nm. The X-Ray diffraction was recorded by Philips PW 1840 XRD.

3. Result and Discussions

Cadmium telluride thin films were deposited by Flash Evaporation technique, which is a very simple and convenient technique. As very little information was available on the deposition of CdTe by this technique, a careful study was undertaken on the various parameters involved in the deposition of CdTe thin films. For the deposition of CdTe films by the 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, proper selection and control of the evaporation boat and substrate temperature provide adequate control of the stoichiometry of the films. Here a very small quantity of the CdTe material was dropped

into the pre-heated 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 substrates 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. The 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 evaporant material fed into the boat through this hole was minimum is shown in Fig.1 . This particular design of boat was found to almost prevent splattering and preferential loss of the more volatile components. CdTe thin films were grown by flash evaporation technique after suitable optimisation of various deposition conditions in the vacuum chamber.

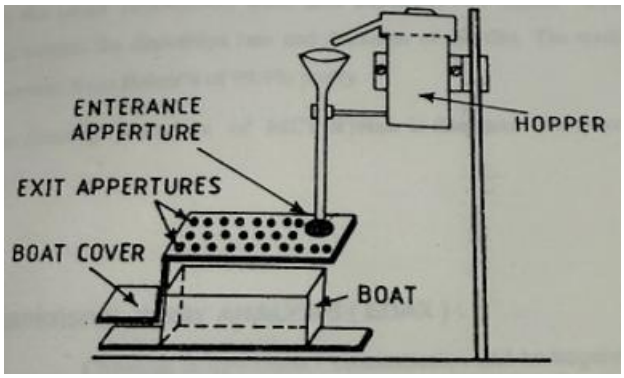

Figure 1: Diagram of the boat used for Flash Evaporation. The Top Cover and the boat hole were locked during operation

Energy dispersive X-ray analysis (EDAX) showed that the composition of resulting CdTe thin film was the same as that of the starting material. The XRD patterns of the CdTe thin films deposited on glass substrates confirmed the Zincblende structure of the CdTe thin film (Fig.3) as well as the source material as shown in Fig 2.

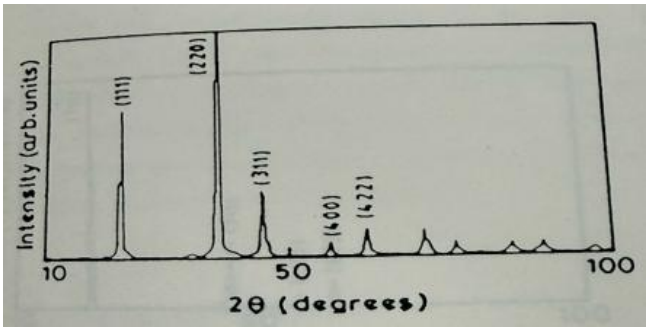

Figure 2: XRD pattern of CdTe Source Material

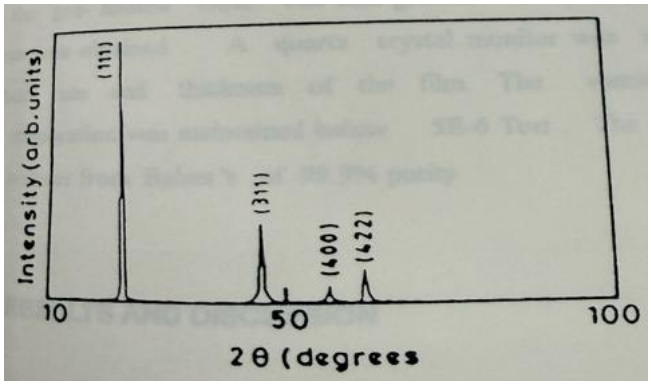

Figure 3: XRD Pattern of CdTe Thin Film

Room temperature resistivity of the CdTe thin films annealed in hydrogen atmosphere showed an increase from $1.5x10^4$ ohm-cm to $9.4x10^4$ ohm-cm as the annealing temperature was increased from 100°C to 250°C. The resistivity showed a sharp increase of four orders of magnitude, i.e. from ~10^4 to ~10^8 as the measuring temperature was decreased from room temperature to 77K. A set of CdTe thin films deposited on a mica substrate were subjected to annealing in hydrogen atmosphere at 80°C in presence of UV photons. During the process, hydrogen was directly passed into the chamber. All the resistivity versus temperature plots of CdTe thin films annealed for different durations, varied from 0h to 4h, showed an increase in resistivity with a decrease in temperature of measurement The resistivity measurements showed an increase from 400K to 50K. The resistivity measurements showed an increase from $2.4 x10^4$ ohm-cm to $3.23 x10^5$ ohm-cm at room temperature, whereas at 77K the resistivity increased from $1.03x10^6$ ohm-cm to $9 x10^6$ ohm-cm, when the annealing duration in hydrogen was increased from 0h to 4h. The value of activation energy as calculated for these films from In p Vs.1/T plots have been found to decrease with annealing time duration both in low-temperature and high-temperature regions Table .3.

Table 1

S. No.	Annealing Duration in H_2 without employing Hg tub (hours)	Band Gap (eV)
1	0	1.435
2	1	1.44
3	2	1.45
4	3	1.46
5	4	1.495

Table 2

S. No.	Annealing Duration in H_2 without employing Hg tub (hours)	Band Gap (eV)
1	0	1.430
2	1	1.415
3	2	1.40
4	3	1.397

Table 3

S. No.	Annealing time (hours)	Activation Energy Region -1 (eV)	Activation Energy Region -2 (eV)
1	With out Annealing	0.0446	0.00416
2	1	0.03932	0.00330
3	2	0.03905	0.003232
4	3	0.02990	0.003017
5	4	0.00398	0.001293

Another set of CdTe films deposited on quartz were annealed in hydrogen atmosphere at 80°C in the presence of UV photons but during this process hydrogen was bubbled through a Hg boat maintained at 100°C. The resistivity measurements carried out at room temperature showed a decrease from $2.4x10^4$ ohm-cm for the unannealed samples to $2.4x10^3$ohm-cm for the samples subjected to annealing for 3hours in a hydrogen atmosphere. For the CdTe thin films annealed in H_2 atmosphere at 80°C in presence of UV photons, where hydrogen was directly passed into the chamber during the process, the optical band gap was also computed from the absorption spectra and was observed to increase from 1.435eV to 1.495eV with an increase in annealing duration from 0hour to 4hour Table 1 . Whereas in the annealing process (at 80°C in the 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 from 1.430eV to 1.397eV with increase in annealing duration from 0hour to 3 hours, which corroborates with the decrease in resistivity with increase in annealing duration, when H_2 was bubbled through Hg boat Table.2 .The CdTe thin films after annealing in hydrogen at 80°C in presence of UV photons. Where hydrogen is directly passed into the chamber shows improvement in the band gap, and also a decrease in activation energy. This shows improvement in crystallinity (17-21) and short range order in films and also dangling bonds may be assumed to be satisfied, resulting in a low value of Value of activation energy.

Conclusions: CdTe thin films suitable for HgCdTe passivation were successfully deposited using the flash evaporation technique after optimization of deposition parameters. Structural studies confirmed the zinc-blende phase and stoichiometric composition of the films. Photothermal annealing in a hydrogen atmosphere significantly modified the electrical and optical properties of the CdTe thin films. Hydrogen annealing increased the resistivity and optical band gap, indicating improvement in film quality and defect reduction. The results demonstrate that optimised CdTe thin films are a promising material for HgCdTe infrared detector passivation applications. Optimized CdTe thin films were successfully deposited by flash evaporation under controlled conditions suitable for semiconductor device applications. Structural analysis confirmed phase purity and stoichiometric composition. Photothermal hydrogen annealing significantly modified electrical and optical behavior, indicating reduced defect density and improved film quality. These findings support the use of optimized CdTe thin films as promising passivation layers for HgCdTe infrared detector technologies.

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