

## Abstract

This thesis contains a detailed study of synthesis, crystal growth and characterization of the II-VI semiconductor ZnTe. The compound has been synthesised by microwave heating for the first time from 7 N's purity Zn and Te. The minimum reaction time was determined to be 30 minutes for 15 gms of material as compared to 24 - 48 hours for conventional thermal synthesis. Single crystals of ZnTe of diameter  $\sim 1$  cm were grown by the vertical Bridgman technique from 4 % Te rich melt at 1150 °C. The growth direction was found to be  $\langle 111 \rangle$ . The high quality of the crystals was demonstrated by their transparent orange colour. XRD proved formation of the zincblende phase with lattice constant  $a = 6.106 \text{ \AA}$ . Inductively coupled plasma (ICP) analysis showed Si, In, Cu and Au to be the main impurities present at ppm level. The etch pit density of the crystals was  $6 - 9 \times 10^5 \text{ cm}^{-2}$ .

Optical absorption studies gave a direct band gap of  $2.26 \pm 0.01 \text{ eV}$  at 300 K. Crystals were p-type with resistivity  $8.5 \text{ } \Omega\text{-cm}$ , hole concentration  $1.6 \times 10^{16} \text{ cm}^{-3}$  and mobility  $46 \text{ cm}^2/\text{V.s}$  at 300 K. The temperature dependence of hole concentration could be explained on the basis of one-centre-one-level statistics associated with a four-fold degenerate valence band. The mobility was found to vary with temperature as  $\mu_p \propto T^{-2.7}$  in the temperature range of 120 - 300 K. The compensation was found to be small ( $N_D/N_A = 0.04$ ) compared with values reported by other workers. After annealing the samples in Zn atmosphere at 650 °C for 12 hours, the resistivity, hole concentration and mobility were found to be  $14.5 \text{ } \Omega\text{-cm}$ ,  $8 \times 10^{15} \text{ cm}^{-3}$  and  $54 \text{ cm}^2/\text{V.s}$  respectively at 300 K. The hole mobility in these samples was dominated by LO phonon scattering in the above temperature range.

In-doped crystals were also grown using the same technique. These samples were found to be high resistive ( $\sim 10^6 \text{ } \Omega\text{-cm}$ ) due to self-compensation. An optical band gap of  $2.06 \pm 0.01 \text{ eV}$  was found for ZnTe:In samples. Thermally stimulated current

measurement showed two traps viz. at 412 - 419 meV above the valence band due to the complex  $V_{Zn}^{=}-In_{Zn}^{+}$  and 180 - 200 meV due to the ionization energy of In.

Hydrogen passivation effects in undoped p-ZnTe single crystal were studied by photoluminescence (PL) and photoconductivity (PC) measurements. Hydrogen passivation was carried out in a parallel plate PECVD reactor at a power level of 0.4 W/cm<sup>2</sup> with samples being kept at 250 °C. PL of the as-grown samples showed peaks at 2.06 eV due to  $O_{Te}$ , at 1.47 eV and 1.05 eV due to Cu and at 1.33 eV due to Au impurities. The temperature variation of PL peak intensities was also studied. After 30 minutes of passivation, new peaks at 2.34 eV and 2.19 appeared and at the same time the peak at 2.06 eV decreased sharply. 60 minutes of hydrogen passivation showed strong near band-edge green luminescence associated with a principal bound exciton at 2.37 eV. 90 minutes of passivation caused severe damage to the surface and resulted in sharp decrease of PL intensity. Hydrogenation had very little effect on the impurity-related peaks at 1.47, 1.33 and 1.05 eV. From the position and thermal quenching energies of the PL peaks, a comprehensive energy level scheme has been proposed for the defect and impurity related transitions in ZnTe. The previously unidentified peak at 1.05 eV has been assigned due to Cu I and that at 1.47 eV to Cu II level.

In PC studies,  $\ln I_d$  vs  $1/T$  plot showed activation energies of 120 and 24 meV before passivation. After 60 minutes of hydrogenation, the dark current ( $I_d$ ) decreased by a factor of 70 and showed activation energies of 40 and 18 meV. The Minority carrier lifetime ( $\tau_n$ ) was calculated from the PC gain.  $\tau_n$  was found to go through a maximum of  $4.5 \times 10^{-7}$  sec at 220 K having activation energies of 40 meV for  $T < 220$  K and 404 meV for  $T > 220$  K. After 60 minutes of passivation,  $\tau_n$  remained constant at  $4.5 \times 10^{-7}$  sec for  $T > 220$  K and decreased for  $T < 220$  K with the same activation energy viz. 40 meV.

Thin films of ZnTe were deposited on glass and Si by pulsed laser evaporation at substrate temperatures of 26 °C and 286 °C. XRD studies showed that films deposited at 26 °C were amorphous while those deposited at 286 °C were polycrystalline. X-ray photoelectron spectroscopy (XPS) showed the Zn : Te ratio to be 49.1 : 50.9 for both types of films. The band gap of the films deposited at 286 °C was 2.2 eV. Resistivity

measurements showed that the ZnTe films had low conductivity at 300 K, with  $\sigma = 2.59 \times 10^{-6} \Omega^{-1}\text{cm}^{-1}$  and  $1.09 \times 10^{-3} \Omega^{-1}\text{cm}^{-1}$  for 26 °C and 286 °C deposited films respectively. The temperature variation of conductivity of the films was studied and the activation energies determined. ZnTe/Si heterojunctions were studied by I-V and C-V characteristics. Both the junctions showed rectifying behaviour. Conduction band offset ( $\Delta E_c$ ) and valence band offset ( $\Delta E_v$ ) were found to be 0.56 eV and 0.58 eV for films deposited at 26 °C. For films deposited at 286 °C, the corresponding values were 0.16 eV and 0.98 eV.

Detailed studies on metal-ZnTe Schottky barriers were carried out using In, Ag, Al and Cu. Weak dependence of barrier height on metal work function was observed. The Fermi level was found to be pinned effectively due to Defect Induced Gap States (DIGS). The density of states at the interface was calculated to be  $4.7 \times 10^{13} \text{ states/cm}^2/\text{eV}$ . The effective Richardson constant  $A^{**}$  was determined to be  $72 \pm 6 \text{ A/cm}^2/\text{K}^2$  from the temperature variation of the I-V characteristics. This was found to be matching exactly with the theoretically calculated value for hole effective mass  $m_h^* = 0.6 m_0$ . The highest and lowest barrier heights of 0.99 eV and 0.80 eV were found for In and Cu which had lowest and highest work function respectively. The ideality factor  $n$  was found to be lowest for In and highest for Al contacts. Temperature variation of barrier height was also studied from the C-V characteristics. The interface index  $S_x = \frac{d\phi_{bp}}{d\chi_m}$ , a parameter used to describe the pinning strength of semiconductors was found to be 0.34, for the first time in this material.

Finally InAs/ZnTe heterojunctions were grown by MOVPE. I-V characteristics of the junctions showed rectifying properties.  $1/C^2$  vs  $V$  plot was found to be linear for both polarities of the applied bias. Thus the junctions showed double depletion characteristics. The conduction and valence band offsets of the heterojunction were found to be 0.24 eV and 1.66 eV respectively. A band diagram has been proposed for this heterojunction.