ABSTRACT of the thesis entitled

Role of Thermally Diffused Arsenic from Semi-Insulating GaAs Substrate in Achieving p-type Conductivity in MOCVD Grown ZnO

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Origin of p-type conductivity in arsenic (As) doped zinc oxide thin films, deposited on semi-insulating GaAs (SI-GaAs) substrates by MOCVD technique was studied in this work. Post deposition thermal diffusion of As from SI-GaAs substrates gives rise to p-type conductivity in the films in oxygen ambiance, with an onset annealing temperature of 600 ^{0}C. On further increasing the annealing temperature to 800 ^{0}C, the conductivity converted from p-type to n-type. To investigate the temperature dependent charge transport mechanism in the As doped p-type ZnO films, the dc conductivity has been measured over a wide range of temperature from 300 K to 10 K. Mott's variable range hopping type of conduction was found to be the dominant carrier transport mechanism in the lower temperature region, whereas, at higher temperature it was governed by the thermally activated type of band conduction. The density functional theory (DFT) calculations were carried out on the basis of spin polarized density of states using Vienna *Ab-intio* Simulation Package (VASP) to investigate the origin of p-type conductivity in As doped ZnO. The calculations were performed for pristine ZnO along with four probable chemical states of As, viz. As_O, As_{Zn}, $As_{Zn}–V_{Zn}$, and $As_{Zn}–2V_{Zn}$ in the films. Theoretical calculation suggests the formation of $As_{Zn}–2V_{Zn}$ defect in ZnO to have a room temperature ferromagnetic nature of the system. The samples showed room temperature ferromagnetic ordering on annealing at 600 ^{0}C. X-ray photoelectron spectra indicated the presence of shallow $As_{Zn}–2V_{Zn}$ acceptor states in the film. The anomaly in the change in conductivity (from p-type to n-type) after further annealing at a temperature of 800 ^{0}C was investigated by using X-ray photoelectron spectroscopic and secondary ion mass spectroscopic techniques. Spectroscopic analysis showed that Ga atoms diffused more than As atoms and substitute Zn atoms thereby forming shallow donor complex, Ga_{Zn}. Electrons from donor levels (Ga_{Zn}) then compensate the holes from acceptor states ($As_{Zn}–2V_{Zn}$) and the material reverts back to n-type. Thus the conversion of carrier type took place due to charge compensation between the donors and acceptors in annealed ZnO/SI-GaAs.

Keywords: Thermal diffusion, Charge compensation, Hopping, DFT.