Proc. of the Intl. Conf. on Nanotechnology for Better Living, 2016
Editors K. K. Kar, A. Shah and R. Sharma
Vol. 3, No. 1, p. 131
doi:10.3850/978-981-09-7519-7nbl16-rps-131

Optical property and defect studies in (Li, Mn) doped ZnO

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ZnO is a wide bandgap semiconductor, categorized in the class of II-VI compound semiconductors, with large values of excitonic binding energy (~60 meV) and bandgap (~3.37 eV) which makes it an ideal candidate for optoelectronic device applications [1].Due to the presence of donor-type defects, like oxygen vacancies, Zn-interstitials and Zn-antisites, ZnO shows n-type behaviour. The intriguing doping study in ZnO has been an extensively discussed area and still throws many open questions for researchers to explore. Especially, realization of p-type ZnO by doping is very difficult and challenging as the native defects in the ZnO lattice compensate the effect of doped acceptor ions. Among many methods proposed to overcome this problem, codoping [2] and cluster doping [3] have been widely used. In our group, efforts have been made to realize p-type ZnO using Li,Ni:ZnO [4]. The current study is done on Li (5 mol%) and Mn (2 mol%) doped ZnO, synthesized by solid state route and characterized by powder XRD. For the study of the optical properties, diffuse reflectance spectroscopy (DRS) along with photoluminescence (PL) studies are carried out and to get a clearer picture of the defect distribution positron annihilation studies (PAS) are also done on the system.

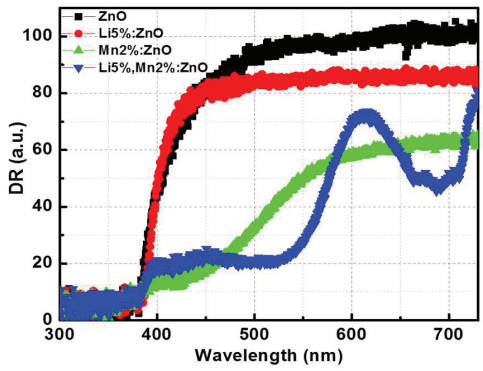

Figure 1: Diffuse reflectance spectra of undoped ZnO, Li 5 mol% ZnO, Mn 2 mol% ZnO, (Li 5%,Mn 2%) ZnO

As can be seen from Figure 1, DRS of undoped ZnO and all the doped samples show absorption edge around 380 nm. In Li doped ZnO bulk sample, only a change in the absorption intensity is observed. In Mn doped ZnO a broad absorption peak centered at around 420 nm is seen which can be attributed to transition between the levels $^6A_1(S) \rightarrow {}^4T_1$ (G) which is formed because of the crystal field effect on the Mn^{2+} ion in tetrahedral coordination in ZnO lattice [5].When ZnO is doped with both Li and Mn, absorption seen around 520 and 687 nm arise (Figure 1 shows diffused reflectance spectra), and these are not related to the transitions due to the crystal field effect on Mn^{2+}. These peaks may be arising from new defect levels created due to the Li-Mn complex formation or formation of complexes between the dopant ions and defects in the lattice. PL spectra for doped ZnO samples (not given here) show a clear suppression of the green luminescence, especially, in (Li, Mn) doped ZnO. This shows that oxygen vacancies responsible for green luminescence are affected by the dopants [1]. As the dopants are expected to occupy Zn sites, this effect can be attributed to the complex formation between the dopants and the oxygen vacancy defects as proposed in the DRS studies. Defect sensitive positron lifetime measurements were carried out on these samples and it was observed that for the undoped ZnO, the positron lifetime is typically 164 ps. Upon doping, the lifetime decreases to 153 ps, which is the bulk lifetime value of ZnO [6]. Further Coincidence Doppler Broadening (CDB) studies are in progress to understand better the reasons for these interesting experimental results and to confirm the kind of complexes formed in the system.

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