Preparation of Mg-doped ZnO nanoparticles by Sol-gel method and their Optical & structural properties

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The optical and structural properties of $Mg_xZn_{1-x}O$ ($0 \leq x \leq 5\%$) synthesized by sol-gel method using the zinc acetate dehydrate Zn $(CH_3COO)_2\,2H_2O$, magnesium acetate Mg $(CH_3COO)_2\,2H_2O$, and citric acid ($C_6H_8O_7.\,H_2O$). These salts were separately dissolved in deionised water keeping cation to citric acid ratio as 1:2. Dissolved salts were further mixed with constant stirring and heated at 100°C till it became viscous solution. This viscous solution was further heated at 120 °C for 12 hours in order to get precursor. This precursor was collected and sintered at 400°C for 1 hour in air by using muffle furnace [1]. The resulting powder was pressed in the form of pellets by applying pressure of 6×10^5 kg/m^2 and then finally sintered at 800 °C for 6 hours.

X-ray diffraction study exhibit the presence of polycrystalline hexagonal wurtzite phase of ZnO for 0-5% of magnesium doping in the host material. Only the shifting of (002) peak towards higher angle side can be observed with the increase in Mg doping as shown in Fig. 1. This is due to smaller ionic radii of Mg^{2+} ion as compared to the Zn^{2+} ion. Similar observation has also been reported by previous studies and the shifting of (002) peak has been correlated with the variation in c parameter [2]. The detailed investigation on the structural properties is performed by estimating the lattice constant, stress, porosity and the crystallite size (D) of the samples. These parameters are estimated by powder-X software [3] and are given in Table 1. Scanning Electron Microscope was employed to analyze the particle morphology and size distribution of the Mg doped ZnO nanoparticles.

Ultraviolet –Visible (Uv-Vis) spectroscope also was employed to analyze the optical absorption of the ZnO nano particles. Tauc plots were used to determine the energy gap of the nanoparticles samples. The optical band gap increases from 3.1 ± 0.1 eV to 3.35 ± 0.1 eV for sample x = 0 to 5%. This increase in band gap may be attributed to the defect states. Change in band gap of the material, there are substantial tails observed towards lower energy side of the absorbance spectra. The tails may be caused by the scattering of a range of particulate sizes or some type of Urbach tail effect due to inter-grain depletion regions. These nanoparticles would be quite useful for their UV LED's applications.

Table 1:c-axis lattice constant (Å), Stress, porosity (P), average crystallite size (D) and Optical band gap of the samples.

Parameters	**ZnO**	**Mg 2%**	**Mg 5%**
c-axis lattice constant (Å)	5.203	5.200	5.198
Stress (GPa)	-3.867	-2.381	-1.712
Porosity (P) (%)	67	66	68
Crystallite Size (nm)	34	39	41
Band gap (eV)	3.10 ± 0.1	3.32 ± 0.1	3.36 ± 0.1

References

1. Fouran Singh, Sanjeev Kumar and A. Kapoor, Journal of Appl. Phys., 112 (2012), 073101.
2. W.Q. Peng, S.C. Qu, G.W. Cong, Z.G. Wang, Appl. Phys. Lett. 88 (2006) 101902.
3. C. Dong, J. Appl. Cryst. 32 (1999) 838.

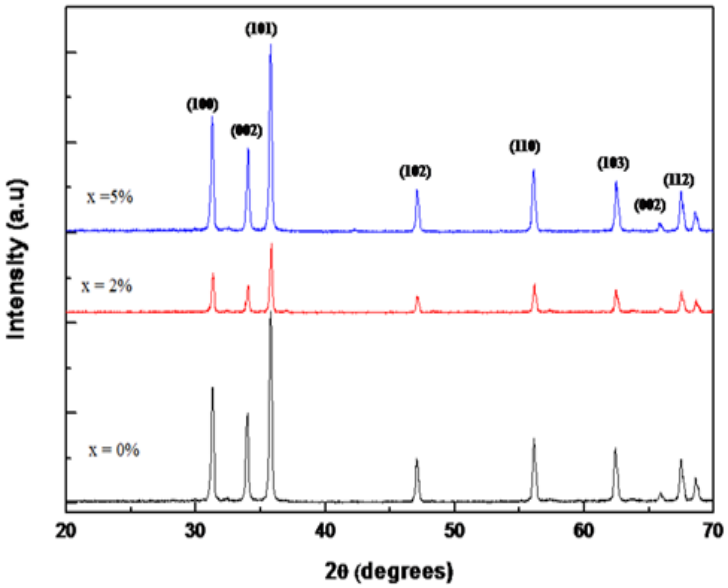

Fig.1: XRD pattern of the $Mg_xZn_{1-x}O$ (x= 0,2,5%) systems

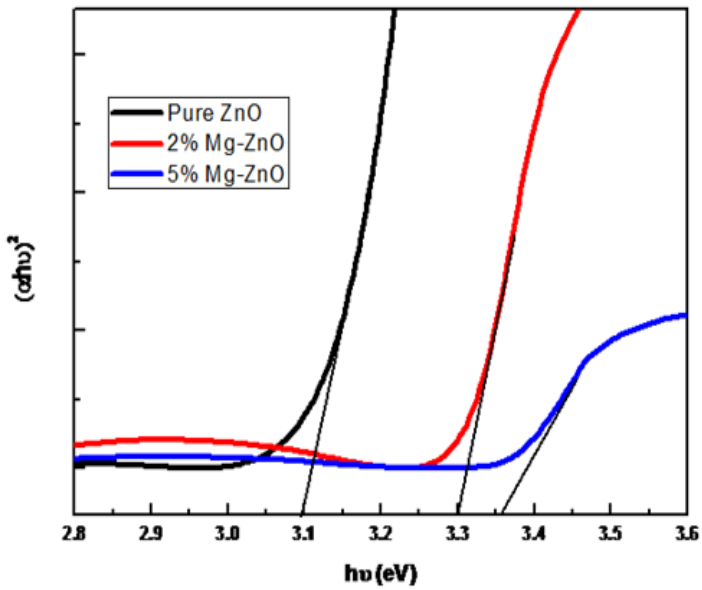

Fig 2: Calculation of band gap of $Mg_xZn_{1-x}O$ (x= 0,2, 5%) by Tauc's Plot method.

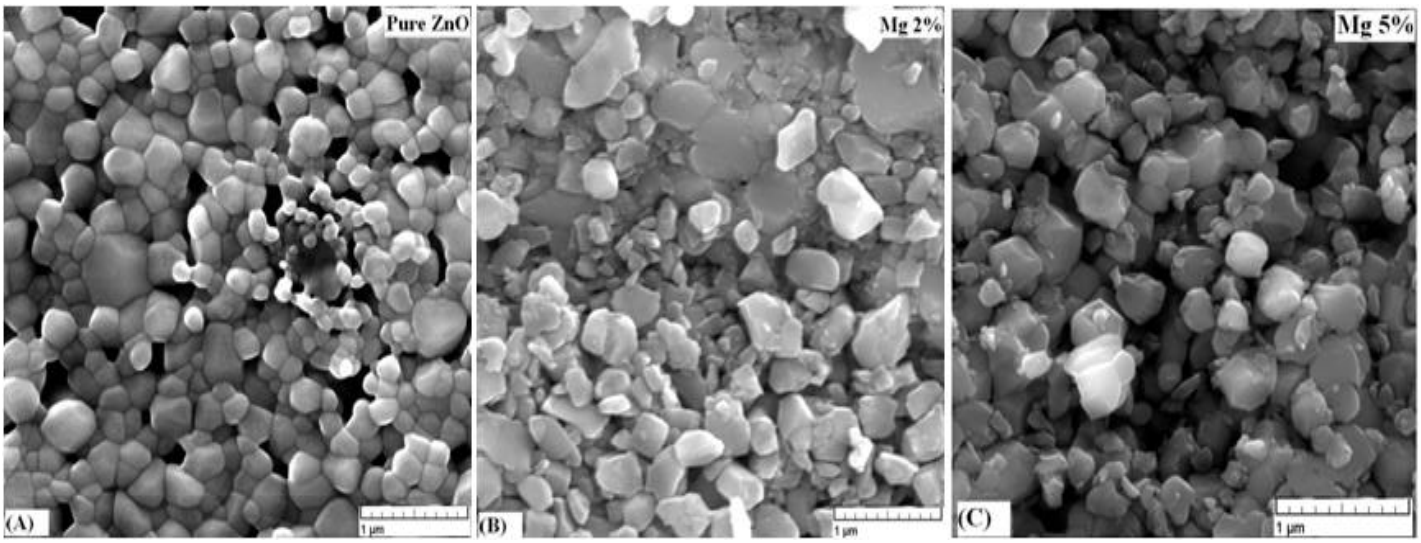

Figure 3: Scanning Electron Microscopy micrographs of $Mg_xZn_{1-x}O$ (x= 0, 2 and 5%) Systems