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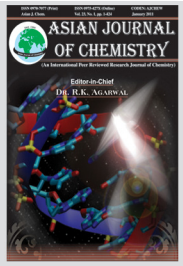

Structural and Optical Properties of Mn Doped ZnO Nanoparticles†

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Manganese doped zinc oxide nanoparticles have been synthesized by the sol-gel method under acid-base reaction followed with pH value 9 to form $Zn_{1-x}Mn_xO$ for different values of x = 0.01, 0.02 and 0.03. The samples are characterized with powder X-ray diffraction and ultraviolet/visible (UV/V) spectroscopy. All samples are found in single phase with polycrystalline nature having wurtzite lattice structure. The UV/V spectra of the nanoparticles indicate a decrease in the band gap from 3.08 eV (for 1 % Mn doped) to 3.05 eV (2 % Mn doped), whereas it increases to 3.11 eV for 3 % doping. The results reveal the lattice strain associated with Mn concentration.

Key Words: Nanomaterials, Zinc oxide nanoparticles, Sol-gel synthesis.

INTRODUCTION

Semiconductors in which cations are partially replaced by transition metal ions are called diluted magnetic semiconductors (DMS)[1]. Strong exchange interactions between external sp carriers of the host semiconductor bands and a localized d electron of the transition metal ion cause interesting spin dependent optical and electrical properties[1]. Since zinc oxide (ZnO) is a wide band gap semiconductor (3.4 eV), ZnO based DMS would be useful for short wavelength magneto-optical applications. It is a promising candidate for the fabrication of gas sensores, piezoelectric transducers and solar cell windows. There has been a lot of interest in doping ZnO with 3d transition metals ions because of potential application in spintronics devises use the spin of electrons in addition to their charge[1]. A few studies have suggested that ZnO doped with transition metals ions could posses interesting optical properties[2-5]. In view of above we have synthesized the Mn doped ZnO with doping concentration x = 0.01, 0.02 and 0.03 and studied their structural and optical properties.

EXPERIMENTAL

The samples of manganese doped zinc oxide ($Zn_{1-x}Mn_xO$) are synthesized by the sol-gel method. Zinc acetate dehydrate $(CH_3COO)_2Zn{\cdot}2H_2O$ and manganese nitrate hydrate have been dissolved in distilled water separately ,then mixed together to get 200 mL volume with molarities of 0.6 M in different values of x = 0.01, 0.02 and 0.03 g, the solution is stirred with a magnetic stirrer adding ammonia to protect the reaction group, the ammonia is added drop by drop until we get pH value 9 at room temperature to yield clear and homogenous gel then centrifuge it with 17300 rpm for a period of 10 s and then kept in a oven at 100 °C .Finally we grind the samples and kept in a furnace at 400 °C for 12 h. The XRD patterns of $Zn_{1-X}Mn_XO$ (x = 0.01, 0.02 and 0.03) samples are recorded with Rigaku Minifex X-ray diffractometer in 2θ range of 20-80 degrees.

The absorption spectra are recorded using Perkin-Elmer λ 35 UV/VIS/NIR system with main and second sample compartment so the spectrum was recorded by taking the main sample as reference and hence transmission due to the second sample only was obtained, the sample was run using SBW 2 nm for wavelength range from 800 to 250 nm with data interval of 1 nm. The spectra were recorded in absorbance *vs.* wavelength plots.

The XRD patterns of $Zn_{1-x}Mn_xO$ (x = 0.01, 0.02 and 0.03) samples are shown in Fig. 1. All the patterns are found to have hexagonal wurtzite structure without any additional impurity phases; it means that the wurtzite structure is not affected by Mn doping. Moreover, as no extra peaks are detected, indicating that all the constituent precursors have been completely decomposed. Further, the 2θ values of the most intense peak are not altered with the increase in the Mn concentration. Lattice parameters are determined using PowderX software and are

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TABLE-1
SOME PARAMETERS OF $Zn_{1-x}Mn_xO$ (x = 0.1, 0.2 AND 0.3) OBTAINED FROM X-RAY DIFFRACTION AND UV/V SPECTROSCOPY

Mn concentration	Crystallite size (nm)	Lattice parameters		Unit cell volume (Å^3)	Band-Gap (eV)
		a (Å)	c (Å)		
0.01	25.72	3.32	5.26	68.72	3.08
0.02	21.81	3.32	5.30	71.58	3.05
0.03	21.27	3.22	5.31	71.75	3.11

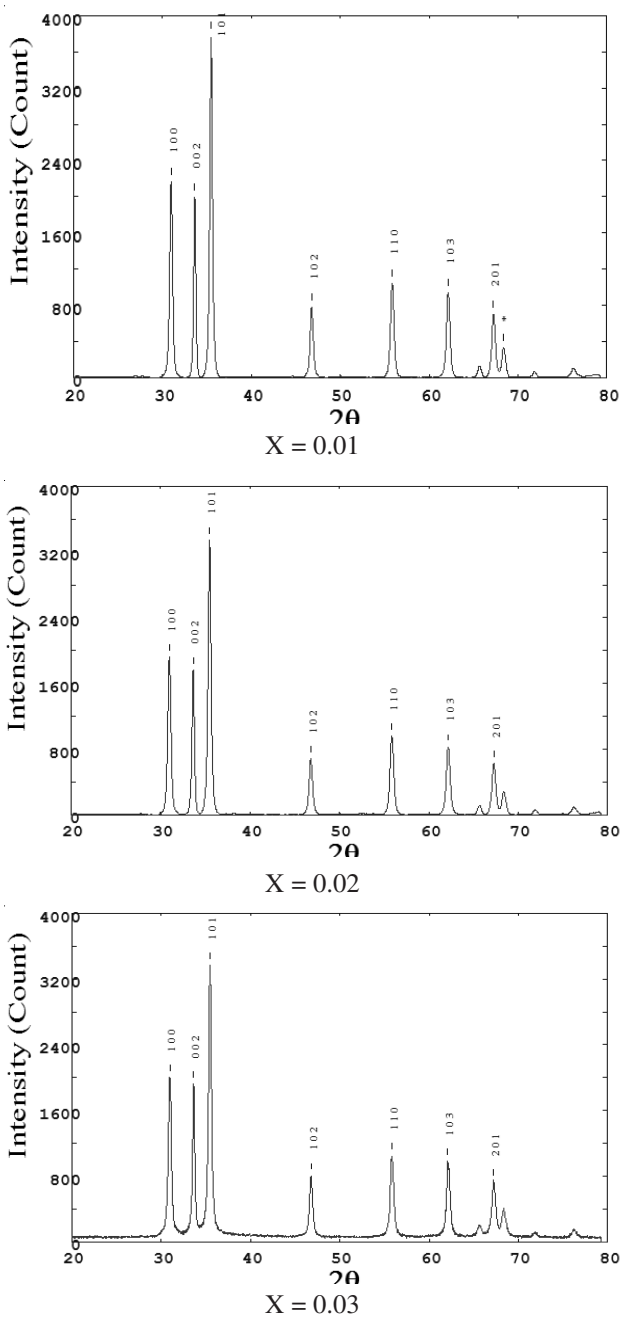

Fig. 1. $(\alpha h\nu)^2$ *versus* hν plots for $Zn_{1-x}Mn_xO$ (x = 0.1,0.2 and 0.3)

found to increase marginally with the increase in Mn concentration. The average crystallite size of the samples is estimated using a (101) peak broadening technique and are formed to be in the range of 20-25 nm as tabulated in Table-1.

In the semi-conducting materials, the optical band gap (Eg) is defined as the energy where the absorption coefficient has a value >10^4 cm^{-1}. In order to find the value of E_g for our samples we make use of the Tauc relation.

$$\alpha h\nu = A (h\nu - E_g)^m$$

where a is absorption coefficient given by $\alpha = 2.303 \log (T/d)$ (d is the thickness of the sample and T is the transmission coefficient), hν is the photon energy.

Fig. 2 shows the plots of $(\alpha h\nu)^2$ *versus* hν for all the samples under investigation. The values of E_g have been estimated by taking the intercept of the extrapolation to zero absorption with photon energy axis *i.e.* $(ah\nu)^2 \rightarrow 0$.

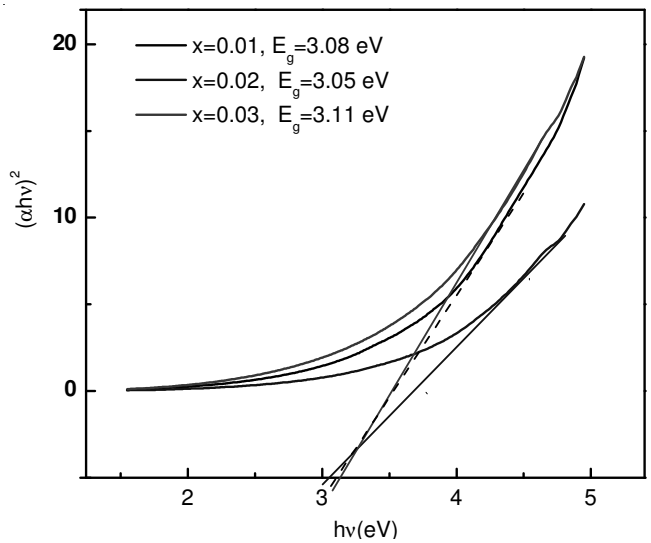

Fig. 2. X-ray diffraction patters of $Zn_{1-x}Mn_xO$ (x = 0.1,0.2 and 0.3) recorded at room temperature

RESULTS AND DISCUSSION

(E_g) is found to be 3.08 eV for 1 % Mn doping and decreases to 3.05 for 2 % .But further increase in Mn concentration results in increase of band gap. Maiti *et al.*[6] also reported the same type of variation in energy gap with the Mn doping. This change in the value of E_g depends on several factors such as grain size, carrier concentration, lattice strain *etc*. But for these samples we assume the lattice strain changes with the Mn doping and hence reflected as the variation of energy gap.

Conclusion

We have studied the effect of Mn doping on structural and optical properties of ZnO. Lattice parameters are found to increase marginally with the Mn doping.

The band gap energy value decrease with increase in doped manganese concentration upto doped manganese concentration x = 0.02 thin it increase for x = 0.03 shows a decrease with the increase in Mn doping up to 2 % but further increase in Mn doping results in the increase of band gap.

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