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Band-Gap Tailoring of Z_nO nanostructures by Mg Incorporation

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Abstract: As Z_nO light-emitting devices have been operated by using ZnMgO layers as energy barrier layers to confine the carriers, it is essential to realize the synthesis and characterization of ZnMgO particularly. In this pursuit, $Zn_{x-1}Mg_xO$ nanostructures have been synthesized using a simple two step thermal decomposition route at high level concentration of Mg (x=0.0, 0.1, 0.2, 0.3, 0.4). Zinc Magnesium Hydroxy Carbonate using varied Magnesium salt concentration was synthesized as precursor for ZnMgO nanostructures. Sudden transformation of these mixed precursors into $Zn_{1-x}Mg_xO$ ternary systems is non-equilibrium process and $Zn_{1-x}Mg_xO$ ternary systems have been synthesized beyond solubility limit of ZnO/MgO. The X-ray diffraction (XRD), Scanning Electron Microscopy (SEM), UV-visible spectroscopy and Photoluminescence spectroscopy (PL) of as synthesized samples have been performed for structural and optical investigation. The variation of lattice constant and the blue shift of near-band-edge emission indicate that Zn^{2+} ions are successfully substituted by Mg^{2+} ions in the ZnO lattice. A decrease in particle size from 19.6 nm to 14.5 nm is observed due to Mg incorporation. Photoluminescence spectra shows the modification in defect structure of ZnO nanostructures by Mg incorporation.

Keywords: ZnMgO nanostructures • Light-emitting devices • Ternary systems • Energy barrier layers

Introduction:

As a wide band semiconductor with large binding energy (about 60meV), ZnO is a promising candidate semiconductor material for the next generation of optoelectronic, light emission or high power and high frequency devices (Pandey et al 2021, Chekroun et al). A crucial step in designing modern optoelectronic devices is the realization of band-gap engineering to create barrier layers and quantum wells in device heterostructures. Alloying ZnO phase with MgO or CdO has been investigated for tuning the band-gap of ZnO based materials (Srinivasa Rao et al 2018, Hsu et al 2006, Mahroug et al 2019). By alloying with MgO, a broader direct band-gap of 7.7 eV, the band gap of ZnO can be remarkably blue-shifted.

Recently, the research of low-dimensional semiconductor nanostructures has been one of the most attractive topics in physics, chemistry and materials science due to their significance in both fundamental and technological fields (Gottardo et al 2021). Interestingly, a diverse range of nanostructural configurations of ZnO including quantum dots, nanobelts, nanorings, nanosprings, nanobows, nanohelices, nanocages, nanowires, nanospheres and microcheerios have been reported. Nanostructured $Zn_{1-x}Mg_xO$ is desired in constructing nanoscale ZnO-based heterostructures.

Although, the thermodynamic solubility limit of MgO in ZnO is only about 4% as suggested by the phase diagram of MgO-ZnO binary system (Linganaboina et al 2018), $Zn_{1-x}Mg_xO$ ternary systems have been synthesized by a number of physical and chemical methods (Hsu et al 2006).

In the present chapter, thermal decomposition method has been chosen to synthesize $Zn_{1-x}Mg_xO$ ternary nanostructures. $Zn_{1-x}Mg_xO$ ternary nanostructures have been synthesized by thermal decomposition of Zn-Mg Hydroxide Carbonate. Sudden transformation of these mixed precursors into $Zn_{1-x}Mg_xO$ ternary systems is non-equilibrium process and $Zn_{1-x}Mg_xO$ ternary systems can be synthesize beyond solubility limit of ZnO/MgO. Here, modification of defect related visible emission by Mg incorporation has been reported in addition to band gap widening.

Material and Methods:

Chemicals:

Zinc Nitrate hexahydrate $[Zn(NO_3)_2.6H_2O]$, Magnesium Nitrate hexahydrate $[Mg(NO_3)_2.6H_2O]$, anhydrous ammonium carbonate $[(NH_4)_2CO_3]$ and Urea from Merck (Mumbai, India) were used as starting material. All the chemicals were of analytic grade and used as received without any further purification.

Sample Preparation:

According to stoichiometric ratio, 50 ml aqueous solution of ammonium carbonate was added drop-wise into the aqueous solution of zinc nitrate and magnesium nitrate. As prepared Zinc-hydroxy carbonate precursor was filtered, washed thoroughly with distilled water, and then dried at 100^0C. The thermal decomposition of Zinc-hydroxy carbonate precursor was carried out at 300^0C for 2 hrs in air atmosphere. The concentration of magnesium nitrate was taken as 0%, 20% and 40% molar percentage of zinc nitrate as to form $Zn_{1-x}Mg_xO$ nanostructures with value of x=0, 0.2, 0.4.

Characterization:

All the measurements for characterization were performed at room temperature. The X-ray diffractometry (XRD) for the crystal structure of the dried powder samples was carried out at Rigaku D/MAX-2200 H/PC diffractometer. The optical absorption was examined with Perkin-Elmer Lambda 35 UV-Visible spectrometer. The emission measurements were carried out using 532 and 355 nm wavelengths of Nd- YAG continuous laser (Coherent, Verdi- V5 system) and Nd-YAG pulsed laser (Litron lasers, Nano TRL system), respectively. An iHR320 (Horiba Jobin Yvon) spectrometer was used to disperse and detect the signal.

Results and Discussion:

Phase Analysis:

Figure 1 shows the XRD patterns of $Zn_{1-x}Mg_xO$ (x=0, 0.2, 0.4) nanostructures prepared by the thermal decomposition of Zn-Mg hydroxide carbonate. The peaks could be indexed to a hexagonal wurtzite ZnO structure for all the nanostructures with no other phase indicating these to be polycrystalline and single phase in the entire composition range. Compared to the case of ZnO, diffraction angle of $Zn_{1-x}Mg_xO$ samples shift to larger angle. This indicates that the Zn^{2+} ions are successfully substituted by Mg^{2+} ions in the lattice. The calculated value of *d*-spacing, *a* and *c* lattice parameter for $Zn_{1-x}Mg_xO$ (x=0, 0.2, 0.4) ternary systems is given in Table 1. The lattice parameters *a* and *c* are decreased for $Zn_{1-x}Mg_xO$ (x=0, 0.2, 0.4) ternary systems in comparison to ZnO. This is quite expected according to vegard's law, as the ionic radius of Mg^{2+} is smaller than Zn^{2+}. A slight increase in lattice parameters is observed for $Zn_{1-x}Mg_xO$ (x= 0.4) in comparison to $Zn_{1-x}Mg_xO$ (x=0.2) ternary system. This indicates that regular Mg substitution occurs only up to x=0.2. According to the phase diagram of the ZnO/MgO binary system, the thermodynamic solid solubility of MgO in ZnO is less than 4 mol % (Hsu et al 2006). In addition, ZnO has a wurtzite structural (*a* = 3.24 Å and *c* = 5.20 Å), while MgO has a cubic structure (*a* = 4.24 Å). This may result in non-equilibrium phase in $Zn_{1-x}Mg_xO$ for higher values of x beyond the solubility limit.

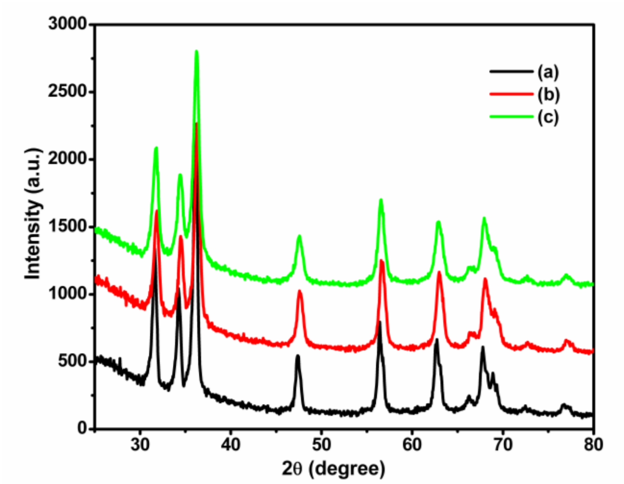

Fig 1. XRD patterns of $Zn_{1-x}Mg_xO$ nanostructures (a) x=0, (b) x=0.2, and (c) x=0.4

Table 1 (101) peak shift, *d*-spacing, *a* and *c* lattice parameter calculated for $Zn_{1-x}Mg_xO$ (x=0, 0.2, 0.4)

	(101) peak shift (^{0}C)	*d*-spacing (Å)	Lattice parameter *a* (Å)	Lattice parameter *c* (Å)
ZnO	36.1032	2.4861	3.2493	5.2964
$Zn_{1-x}Mg_xO$, x=0.2	36.3024	2.4729	3.2321	5.2683
$Zn_{1-x}Mg_xO$, x=0.4	36.2262	2.4779	3.2387	5.2790

Also the XRD pattern shows the peak broadening upon the incorporation of Mg^{2+}. This may correspond to the reduction in particle size. The replacement of Zn by Mg will affect the lattice and induces internal strain which in turn suppress the grain growth. The particle size calculated by using Scherrer's formula is 19.6 nm, 14.7nm and 14.5 nm for ZnO, $Zn_{1-x}Mg_xO$ (x=0.2) and $Zn_{1-x}Mg_xO$ (x=0.4), respectively.

SEM Analysis

The SEM analysis (shown in figure 2) show that the microstructure of ternary systems is highly influenced by the content of magnesium in the sample.

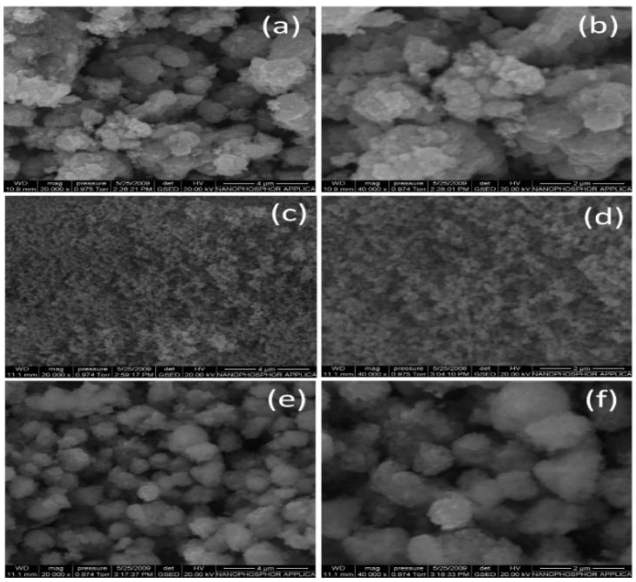

Fig 2 SEM images of $Zn_{1-x}Mg_xO$ nanostructures for x=0 (a),(b) x=0.2 (c),(d), and x=0.4(e),(f)

UV-visible Spectroscopy

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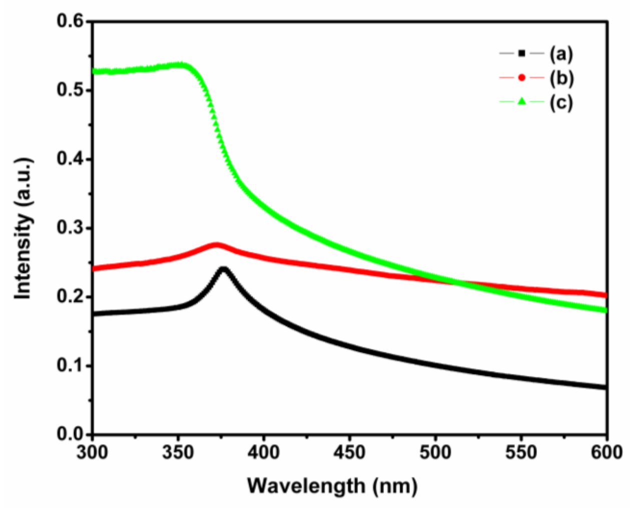

Fig 3. UV-visible spectra of $Zn_{1-x}Mg_xO$ nanostructures (a) x=0, (b) x=0.2, and (c) x=0.4

Figure 3 shows the optical absorption spectra of $Zn_{1-x}Mg_xO$ nanostructures (x=0.0, 0.2, 0.4). The excitonic nature of the absorption spectra is clearly visible in the spectra. The absorption edge is blue-shifted from 376 nm for $Zn_{1-x}Mg_xO$ (x=0) to 354 nm for $Zn_{1-x}Mg_xO$ (x=0.2). This explains the broadening of ZnO by Mg incorporation (Hsu et al 2006, Ercan et al 2022).

Photoluminescence Spectroscopy

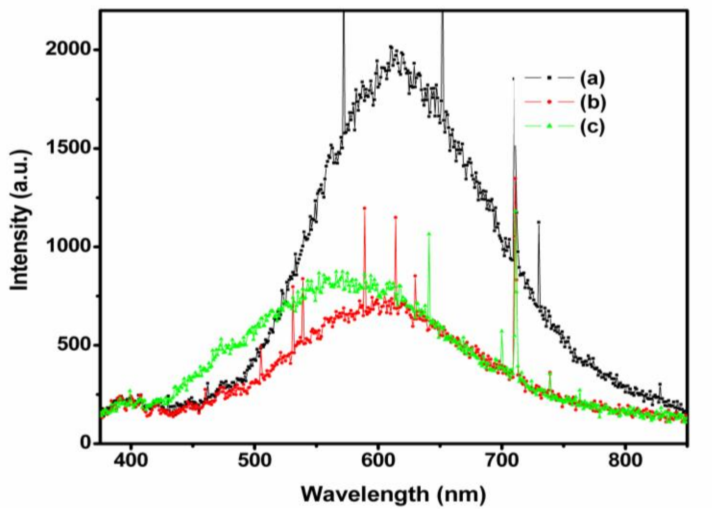

Fig 4. Photoluminescence spectra of $Zn_{1-x}Mg_xO$ nanostructure x=0 (a), 0.2 (b), 0.4 (c)

The room temperature photoluminescence spectra of $Zn_{1-x}Mg_xO$ nanostructure (x=0, 0.2, 0.4) under 355 laser excitation is shown in figure 4. The pure ZnO nanostructure shows broad red emission and can be correlated to single negatively charged interstitial oxygen ion (O^-_i). A blue shifting and broadening is observed by magnesium incorporation. Also the photoluminescence intensity decreases on increasing Mg concentration. The blue shift and broadening can be explained as introduction of more defect level on the high energy side by the incorporation of magnesium (Lewis et al 2022, Zhou et al 2022, Chawla et al 2008, Linganaboina et al 2024).

Conclusions:

The study shows the successful synthesis of ZnMgO nanostructures at higher concentration of Magnesium by using a simple thermal decomposition method. XRD and SEM analysis shows high quality of synthesized

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ZnMgO nanostructures. The chosen synthesis method promotes uniform growth of nanostructures with controlled particle size of range 19.6 nm to 14.5 nm. The optical spectra of samples show the widening of band-gap of ZnO nanostructures by Magnesium incorporation. In addition, photoluminescence study shows that the careful incorporation of Mg in ZnO nanostructures have ability to modify defect structure of ZnO nanostructures in such a way that it can be developed as phosphor material for white light emitting diodes.

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