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Preparation and characterization of Barium Incorporated Zinc Oxide nanoparticles

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Abstract : Pure ZnO and Ba dopped ZnO nanoparticles can be prepared by sol gel method. The procedure for the preparation of BaZnO nanoparticles are discussed in detail. The synthesis particles were subjected to UV-Visible, FTIR, XRD, SEM with EDS. The obtained results from the above characterization techniques are interpreted with the available literatures.

Introduction

Introduction ZnO is the hardest of the II-VI semiconductors due to the higher melting point (2248k) and large cohesive energy (1.89ev) (therefore more resistant to wear), as well as one of the most piezoelectric semiconductors (d= 12.2 × 10-12 C/N) with good piezoelectric coefficient KL =0.27 and its high adherence on various substrates[1-4]. Moreover it is used in a variety of technical applications, including porcelain enamels, heat resisting glass, an activator in vulcanization, an additive for rubber and plastics, pigment in paints with UV protective and fungi static properties, spacecraft protective coatings, a constituent of cigarette filters, healing ointments, in optical waveguide, and many more [5]. ZnO has played an important role in the fabrication of transparent thin film transistors (TFT), by depositing channel layer on a flexible substrate through low temperature processes, realizing transparent TFTs, and achieving extra functions such as photo detections using ZnO channel. In this case the protective covering to prevent light exposure is eliminated since ZnO based transistors are insensitive to visible light. The deposited ZnO usually maintains a crystalline phase, although the deposition process is carried out even at room temperature [6, 7].

Experimental

ZnO nano powder was synthesis by sol gel process. Zinc acetate [Zn(CH3CO2)2.2H2O] and NaOH were used as a precursor material and the solvent, respectively. Zinc acetate was dissolved in NaOH by the molar ratio of 1:85. After stirring the solution with reflux at 70- 750 C for 4 hours. Then filtration was done by what man filter paper. During the filtration solution was washed by ethanol many times to avoid the impurities. After filtration, filtered sample was heated at 900C in oven for 2 hours. Heated sample was grinded and characterized under many techniques (like XRD, FTIR, SEM, UV etc.)

Results and Discussion

XRD

The XRD patterns of both ZnO and ZnO:Ba nanopowders. As can be seen, all the diffraction peaks match very well to the wurtzite ZnO structure (JCPDS card No. 891397), which diffraction peaks are shown as lines in the lower side of the figure. The strong diffraction peaks indicate that the product exhibits good crystalline.

Morphological Study of Ba doped ZnO Powder

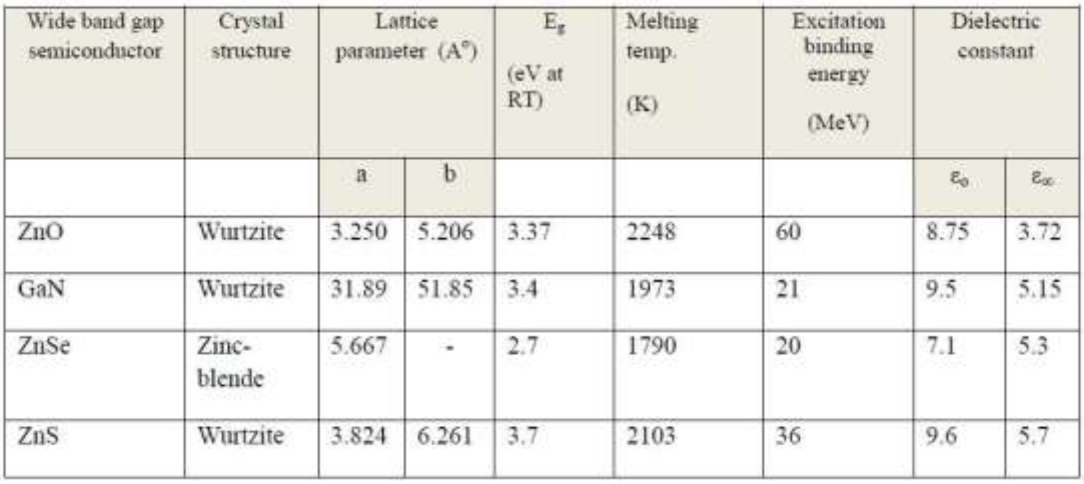
The composition analysis from the EDX spectrum (Fig)shows that the Ba composition in ZnBaO sample is 2.35 at% for Ba doping in ZnO. It is observed that the measured at% of Ba is lesser than the nominal composition values. Therefore it is not easy for Ba ions to enter the ZnO crystal structure, indicating that this ZnO growth process is in equilibrium state, to avoid the inclusions of foreign phases. Fig shows the EDX spectrum of pure and Ba doped ZnO nanopowders.

Table 4.1 gives the ratio of Ba:Mn:O elemental composition. EDX analysis confirmed the presence of manganese in ZnO crystal. Fig. 4.4 shows the SEM images of pure and Mn doped ZnO nanopowders.

UV–Vis absorption spectral study of doped ZnO powder

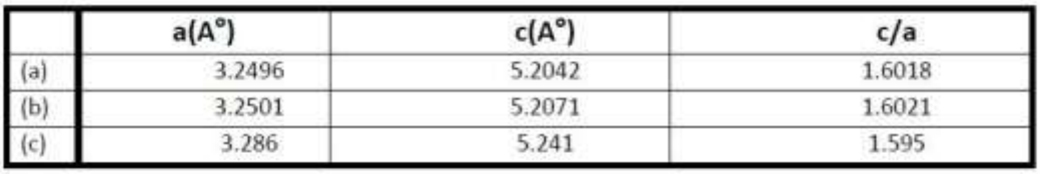
Fig. 4.5 shows the UV–Vis absorption spectra of ZnO with different Mn concentration. The absorption edge of pure ZnO is 190nm and Ba doped ZnO are 199.77 and 208.05nm, respectively. The position of the absorption spectra is observed to shift towards the lower wavelength side with increasing Ba doped concentration in ZnO. This indicates that the band gap of ZnO materiasl increases with the doping concentration of Ba ion. The increase in the band gap or blue shift can be explained by the Burstein–Moss effect [12]. This is the phenomenon on that the Fermi level merges into the conduction band with increase of the carrier concentration. Thus the low energy transitions are blocked.

Table 1.1.Comparison of different semiconductors



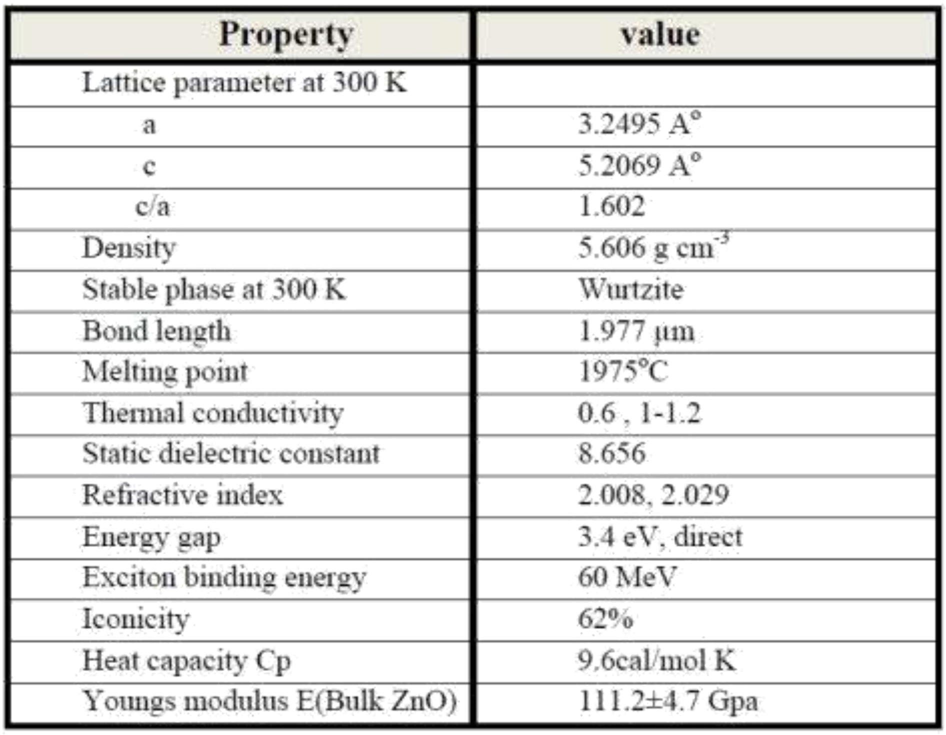
Wide band gap semiconductor	Crystal structure	Lattice parameter (A°)		E_g (eV at RT)	Melting temp. (K)	Excitation binding energy (MeV)	Dielectric constant	
		a	b				ε_0	ε_∞
ZnO	Wurtzite	3.250	5.206	3.37	2248	60	8.75	3.72
GaN	Wurtzite	31.89	51.85	3.4	1973	21	9.5	5.15
ZnSe	Zinc-blende	5.667	-	2.7	1790	20	7.1	5.3
ZnS	Wurtzite	3.824	6.261	3.7	2103	36	9.6	5.7

Table 1.2 Measured and calculated lattice constants.



	a(A°)	c(A°)	c/a
(a)	3.2496	5.2042	1.6018
(b)	3.2501	5.2071	1.6021
(c)	3.286	5.241	1.595

Table 1.3 Basic physical properties of ZnO



Property	value
Lattice parameter at 300 K	
a	3.2495 A°
c	5.2069 A°
c/a	1.602
Density	5.606 g cm^{-3}
Stable phase at 300 K	Wurtzite
Bond length	1.977 µm
Melting point	1975°C
Thermal conductivity	0.6 , 1-1.2
Static dielectric constant	8.656
Refractive index	2.008, 2.029
Energy gap	3.4 eV, direct
Exciton binding energy	60 MeV
Iconicity	62%
Heat capacity Cp	9.6cal/mol K
Youngs modulus E(Bulk ZnO)	111.2±4.7 Gpa

Table 4.1 The ratio of Ba:Mn:O elemental composition

Dopant concentration (at %)	**Experimental results (Atomic %)**		
	Zn	**Ba**	**O**
0	39.51	----	60.49
0.5	41.13	2.35	56.34

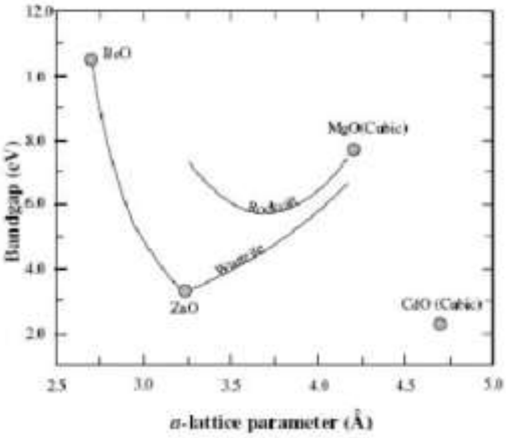


Fig. 1. 2:Band gap vs. in-plane lattice constant for the ternaries

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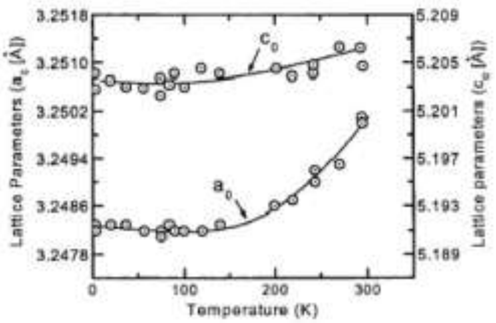


Fig.1.3 Wurtzite ZnO lattice parameters as a function of temperature

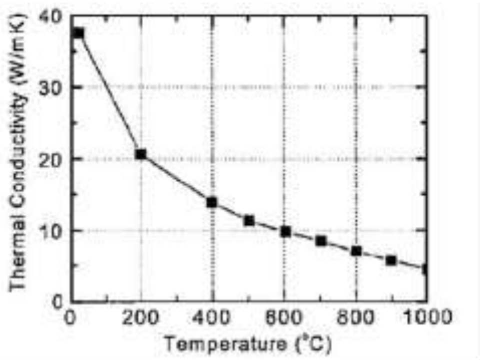


Fig.1.4 Thermal conductivity of fully sintered ZnO heated from room temperature to 1000 °C

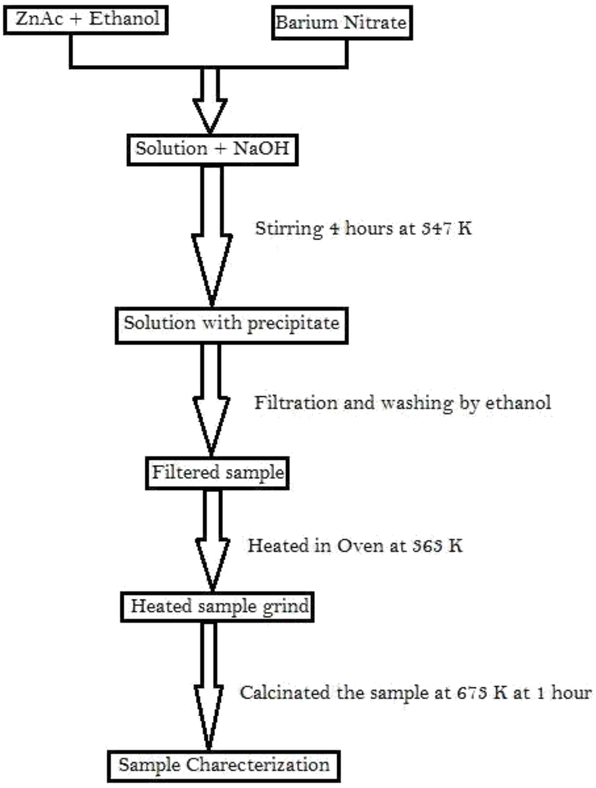


Fig.3.1 Synthesis of ZnO nanopowder by sol-gel route

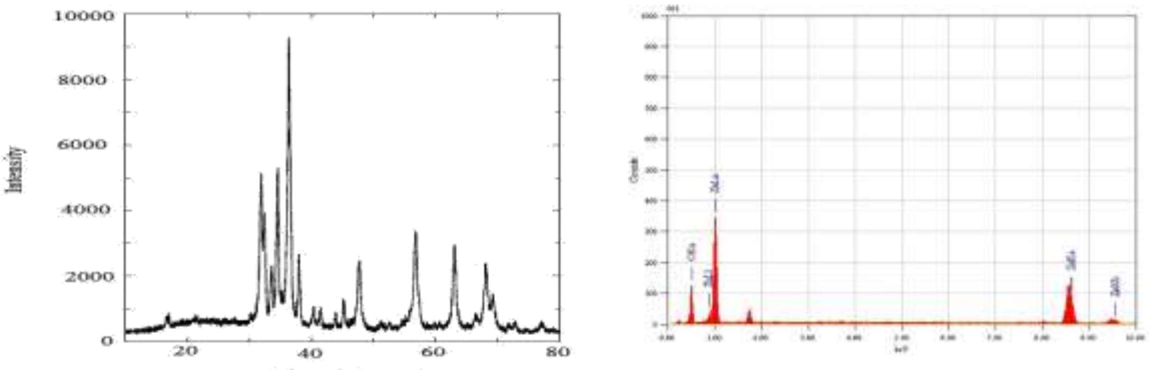
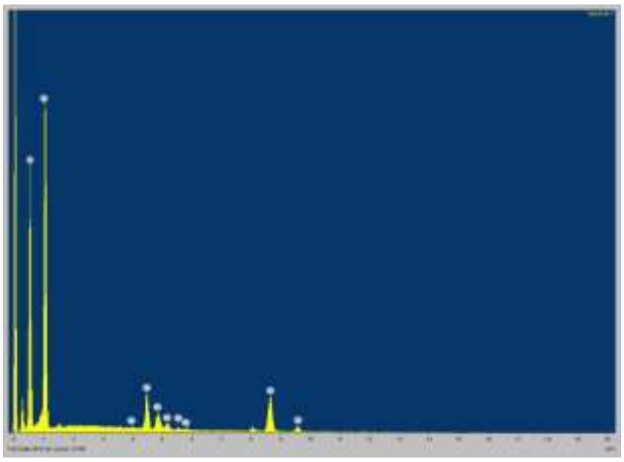


Fig. 4.2 X-ray diffraction pattern of Ba doped ZnO Nano powder



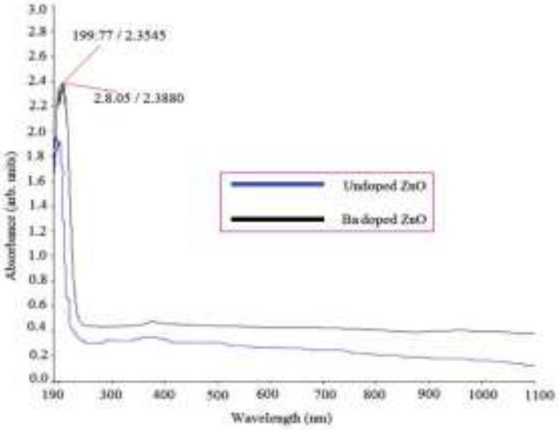
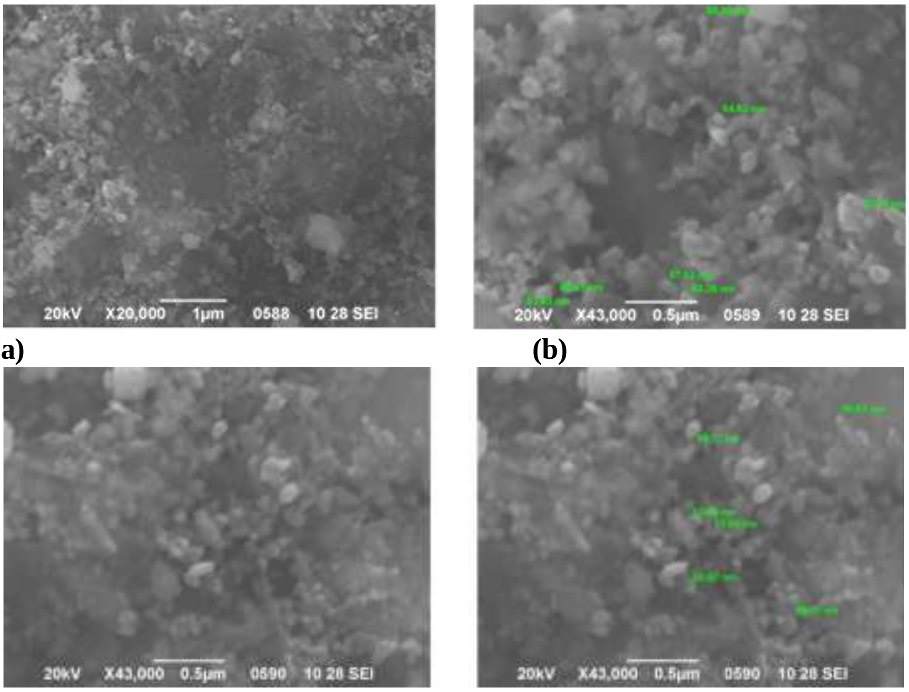


Fig. 4.3 EDX spectrum of Pure and Ba doped ZnO

Fig. 4.5 UV–Vis absorption spectra of pure and Ba doped ZnO



(a) **(b)**

(c) **(d)**

Fig. 4.4 SEM images for (a) pure ZnO, (b)-(d) Ba doped ZnO

Conclusions

Pure Zinc Oxide and Barium dope Zinc Oxide nanopartiles were synthesized by sol-gel technique. The X-ray diffraction patterns were characterized for the purpose of crystal formation. Morphological images were characterized with help of SEM. The average particle size of the doped Zinc Oxide nanopartile is 58-62nm . This was obtained from scanning electron microscopic images of synthesized samples. The optical properties were characterized using UVVis specteral analysis. The absorption edge of pure ZnO is 190nm and Ba doped ZnO are 199.77 and 208.05nm. This result shows dopent materials were increasing the band gap of the material. From this study, we can suggest the doped semiconductor will be used for photacatalytic, gas sensor, solar cell applications.

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