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STRUCTURAL AND MORPHOLOGICAL CHARACTERIZATION OF DOPED ZnO

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ABSTRACT

The bismuth tri oxide doped ZnO was prepared by solution combustion method and annealed at 600^{0}C. The structural,morphological and the chemical composition were studied using XRD,SEM and FTIR. Absorption spectra studies were carried out by UV Visible Spectroscopy. The particle size with the doping concentration is calculated. The reduced particle size influences the electrical properties. The XRD study showed the presence of secondary phases due to the substitution of zinc with other cations such as bismuth. The FTIR spectra confirm the chemical bonding and composition of the sample. The presence of bismuth rich and ZnO matrix phase was confirmed by the FESEM. It is recorded that the band gap decreases with increase in particle size.

Keywords: Combustion,doping,cations

I.INTRODUCTION

ZnO is a semiconductor material with direct band gap energy of 3.37eV and high exciton binding energy of 60meV(1).Furthermore ZnO is stable in hydrogen plasma and environment, low cost material and transparent in visible light region(2-5). The ZnO has various application in the areas such as optoelectronics,sensors,transducers and biomedical science(6). Doping with alkali metals can enhance the properties of ZnO(7-11). Commonly used alkali metals including (nitrogen),phosphorous, arsenic and antimony(12-17).Among these Bi_2O_3 possess higher optical performance. The bismuth doped ZnO posses high transmittance(18). The current trends show that the Bi_2O_3 doped ZnO shows various scientific as well as technological applications(19). It show low optical basicity(0.43) and known as strong acidic oxide(20). By knowing the optical basicity it is useful for the design of the novel optical functional materials with higher optical

performance(21). Transparency to near infrared(0.8μm) to far infrared region(2.5 μm) and thus they have photonic applications. It is observed that the Bi_2O_3 is a promising substitute for lead base materials. Thus we can say that it is a very eco-friendly material for various applications such as plasma display panels, glass ceiling,radiation shielding glasses etc.

In this paper, we report the synthesis of Bi doped ZnO and the effect on the structural, morphological and optical properties.

II. EXPERIMENTAL DETAILS

In combustion synthesis, a starting aqueous precursor of metal nitrates such as $Zn(NO_3)_2$ and $Bi(NO_3)_3$ and a suitable organic fuel, glycine (reducer) predetermined in organic ratio. The mixture is stirred well with HNO_3

(oxidizer) and distilled water. On continuous heating itself ignites to produce the product on. Then it is annealed to 600^{o}C by using a muffle furnace. After annealing it appears pale yellow in colour .

$Zn(NO_3)_2 \cdot 6H_2O + x\ Bi(NO_3)_3 \cdot 6H_2O \rightarrow Zn_{(1-x)}Bi_xO$

+ gaseous products (1)

The scanning electron microscopy is used to find out the morphological study. Phase analysis and crystal geometry of nanoparticles can be measured with Bruker AXS D8 Advance with Cu target radiation (λ =1.5406 A^{0}). Fourier transform infrared analysis was carried out by using IR Prestige-21. UV-Visible spectrophotometer is used to find out the band gap.

III. RESULTS AND DISCUSSIONS

3.1 X-RAY Diffraction

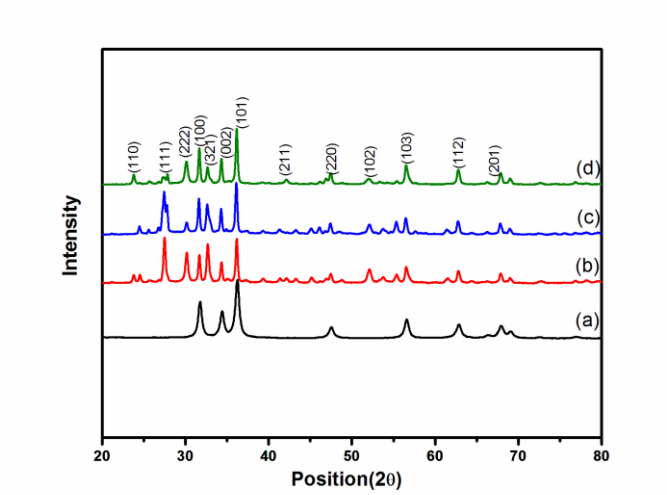

Fig 1.XRD pattern of (a) ZnO (b) Bi $_{(0.1)}$:Zn $_{(0.9)}$ O , (c) Bi $_{(0.15)}$:Zn $_{(0.85)}$ O (d) Bi $_{(0.2)}$:Zn $_{(0.8)}$ O

XRD technique is used to study the crystalline phases and structural properties of nanoparticles. The diffraction peaks at (101),(100),(002),(220),(110) and (103) corresponding to 2θ values 36^{0} 31^{0}, 34^{0}, 47^{0}, 23^{0}, 62^{0} match with standard JCPDS file No. 36-1451of ZnO (Fig.1). It is observed that it possess hexagonal wurtize structure. Additional peaks at (321),(222) and 111) belongs to Bi_2O_3(JCPDS FILE No.65-4020). Crystallite size can be estimated by using the relation:

$$D = \frac{K\lambda}{\beta \cos\theta} \quad (2)$$

Where K is the constant determined by geometry of crystallites and its value approximately equal to 0.9, β is the full width of half maximum. λ is the wave length of X-rays, θ is the glancing angle.

Lattice parameter can be calculated by using the equation:

$$\left[\frac{1}{d_{hkl}}\right]^2 = \frac{4}{3}\left[\frac{h^2+k^2+l^2}{a^2}\right] + \frac{l^2}{c^2} \quad (3)$$

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Table1. Parameters of prepared samples

Sample Details	Lattice parameter (A^0)			Crystallite size D (nm)	Band gap (eV)
	a	C	c/a		
Pure ZnO	3.26	5.25	1.625	39	3.16
$Bi_{(0.1)}:Zn_{(0.9)}O$	3.26	5.18	1.593	25	3.14
$Bi_{(0.15)}:Zn_{(0.85)}O$	3.25	5.09	1.565	26	3.12
$Bi_{(0.2)}:Zn_{(0.8)}O$	3.24	5.08	1.567	27	3.10

From Table 1 it is found that crystallite size of nanoparticles lies in the range of 39-25 nm.

3.2 SCANNING ELECTRON MICROSCOPY

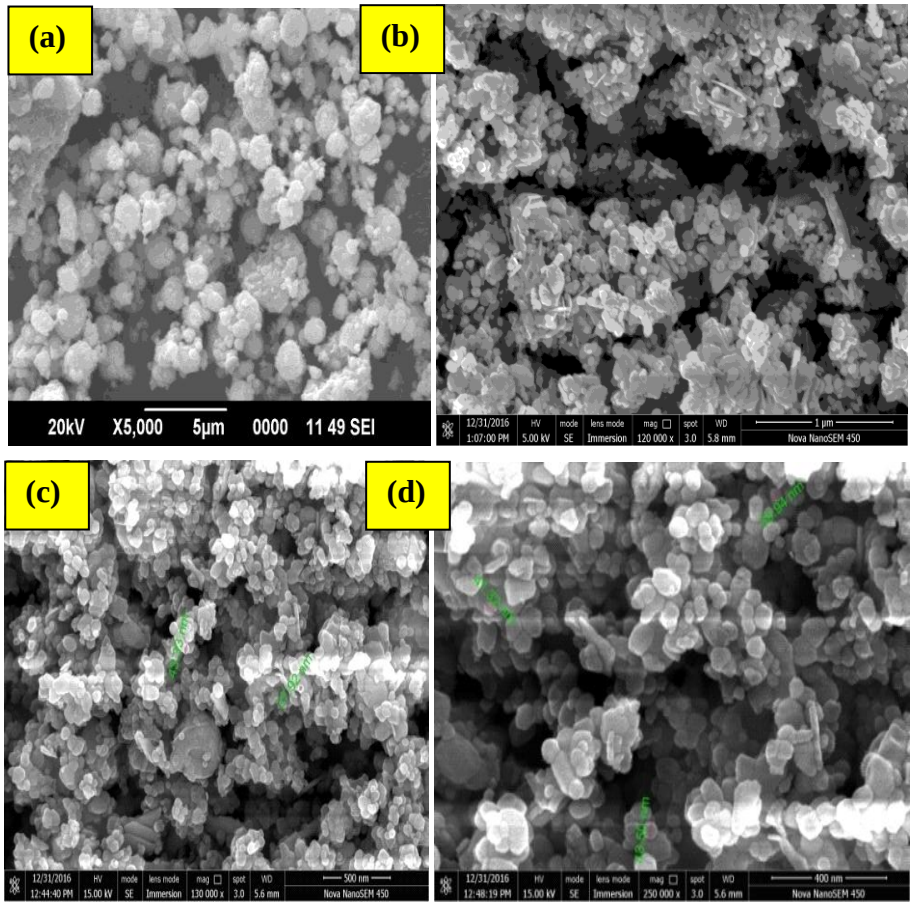

Fig 2.SEM pattern of (a) ZnO (b) $Bi_{(0.1)}:Zn_{(0.9)}O$, (b) $Bi_{(0.15)}:Zn_{(0.85)}O$ (c) $Bi_{(0.2)}:Zn_{(0.8)}O$

The SEM morphology shows that they are cuboid in nature,obtained through combustion synthesis.The overall surface shows the grains and the grain size is also calculated.It more or less covers the whole surface and uniformly covered without cracks.Some holes are present which indicates the presence of porosity.

3.3 FTIR Spectroscopy

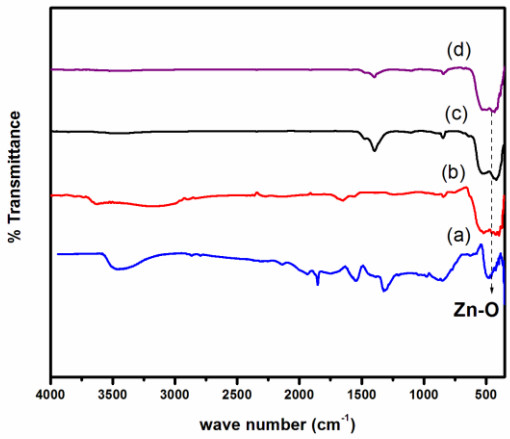

Fig 3.FTIR spectra of (a) ZnO (b) $Bi_{(0.1)}:Zn_{(0.9)}O$, (b) $Bi_{(0.15)}:Zn_{(0.85)}O$ (c) $Bi_{(0.2)}:Zn_{(0.8)}O$

The chemical bonding and the vibrational properties can be recorded by using FTIR spectroscopy.This is based on the absorption of infrared radiation by the material.It is obvious that the band structure and absorption peaks depend upon the morphology of the sample. The FTIR spectrum of Bi_2O_3 doped ZnO in the spectral range of 400-4000cm^{-1} .The broad peak in the range 3219-3570 cm^{-1} for ZnO and 3119-3450cm^{-1} corresponds to symmetrical and asymmetrical stretching vibrational mode of O-H bonds which is attributed to the presence of surface absorbed water molecules.The strong absorption peak around 550cm^{-1} attributed to the Zn-O stretching vibrational bonds. However, the unique peak is observed at 840$cm^{-1}$for the Bi_2O_3 doped ZnO NPs can be assigned to the Bi-O symmetric stretching vibrations in the pyramidal BiO_6 units.

3.4 UV Visible Spectroscopy

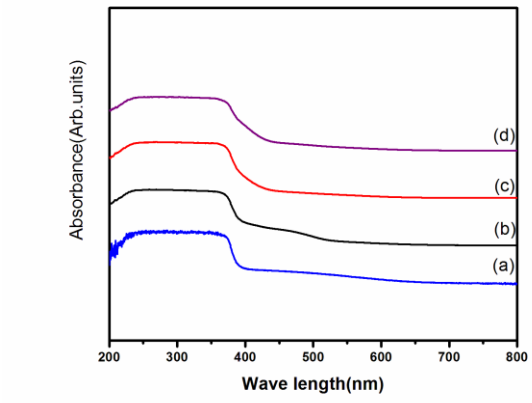

Fig 4.Absorbance s of (a)ZnO (b) $Bi_{(0.1)}:Zn_{(0.9)}O$, (c) $Bi_{(0.15)}:Zn_{(0.85)}O$ (d) $Bi_{(0.2)}:Zn_{(0.8)}O$

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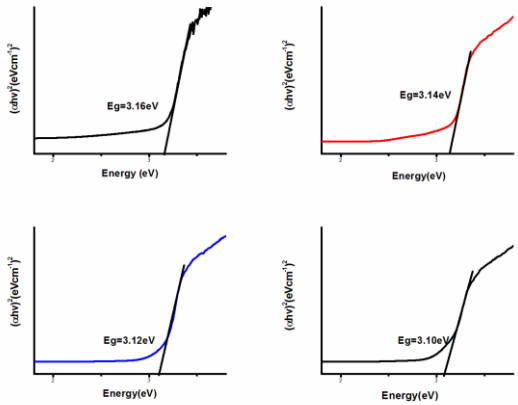

Fig 5.Tauc plot of (a) ZnO (b)Bi $_{(0.1)}$:Zn $_{(0.9)}$ O , (c) Bi $_{(0.15)}$:Zn $_{(0.85)}$ O (d) Bi $_{(0.2)}$:Zn $_{(0.8)}$ O

UV Visible Spectroscopy is carried out to determine the optical properties of nano powders. Absorbance spectra of Bi doped ZnO nanoparticles were shown in Fig 6. Maximum absorbance lies in the range of 300-350 nm.The optical band gap values can be calculated by the following relation:

$$\alpha = A\left(h\nu - E_g\right)^n \qquad (4)$$

where α is the absorption co-efficient, hν the photon energy, A is a constant, E_g is the optical band gap and n is an index that characterizes the optical absorption and it is equal to 2 and 1/2 for indirect and direct allowed transitions, respectively. Band gap can be calculated by using the Tauc plot. Band gap can be estimated by plotting hν versus $(\alpha h\nu)^2$.Extrapolation to energy axis gives corresponding band gap values. Obtained band gap values are shown in Table 1. Reduction in band gap with doping may be due to quantum confinement. Increase in the band gap results the decrease in particle size of nanophosphor materials.

IV. CONCLUSION

Here we have reported the synthesis of Bi doped ZnO by simple solution combustion method. The structural, morphological and optical properties of the sample were recorded using XRD,SEM,FTIR and UV-Visible spectroscopy. By using Scherrer formula we have calculated the average particle size of the sample. From the FTIR spectra the chemical composition and the bonding is also calculated. The morphology can be explained with the help of SEM imaging and the grain size is also calculated. Band gap reduction with increase in doping concentration of Bi make it suitable for optoelectronic applications.

VI. ACKNOWLEDGMENTS

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