

SYNTHESIS AND CHARACTERIZATION OF P₂O₅ DOPED ZnO

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Abstract

ZnO nanoparticles has drawn great attention due to the presence of ZnO which act as a network former or modifier . It offers wide range of application in optoelectronics with a wide band gap 3.37 eV at room temperature. Now a days ZnO nanoparticles has wide range application in optoelectronic devices. The aim of the present study is to prepare P₂O₅ doped ZnO with different concentrations with good structural, morphological and optical properties. The samples were synthesized using solid state reaction method. The structures of the powdered sample were studied using X-Ray Diffraction technique. The chemical groups of the sample were discussed by using FTIR. UV-visible spectroscopy reveals that as the doping increases the band gap decreases and then increases . Photoluminescence (PL) and SEM studies were also carried out.

Keywords: Nanoparticle, Photoluminescence and Band gap.

1.Introduction

Zinc oxide posses an exciton binding energy of 60meV with a wide band gap which leads to possible light emitting applications well above the room temperature¹⁻². It can be applied in the field of optical and electrical devices ,piezo electricity, drug delivery ,solar cell ,cosmetics³⁻⁷. Lack of stable, conductive p-type epitaxial layers due to its asymmetric doping limits strongly against p doping is the major obstacle to the development of P₂O₅-doping is the major obstacle to the development of ZnO⁸.High carrier concentration, reasonable mobility and low resistivity are expressed by P₂O₅ doped ZnO⁹.Because of the unique physical properties such as high thermal expansion coefficient, low melting and softening temperature, high electrical conductivities, extensive UV transmissions P₂O₅ have attracted much attention¹⁰.The structural,physical and chemical durability properties of the host can be modified by ZnO¹¹⁻¹³.

In this paper, we report the synthesis of P₂O₅ doped ZnO and the effect of P₂O₅ on the morphological and optical properties. P₂O₅ doped ZnO compounds could be well acheived in future.

2.Experimental details

The P₂O₅ nano materials with three different concentrations 1 wt%,1.5 wt% and 2 wt% were synthesized by solid state reaction method. ZnO and P₂O₅ are weighed accurately and it is placed in an agate motor. The mixture is grinded with substrate, acetone. Then the mixture is placed in an oven for one hour at 80°C.Again grind the mixture and places it in the oven for one hour at 80°C.Then it is calcined to 600°C by using Muffle furnace and analyzed. The pure ZnO samples were present in the white colour, while P₂O₅ doped ZnO for different concentrations becomes light ash and the colour becomes deeper and deeper with the increasing P₂O₅.



Table 1. Sample code of prepared samples

Sample code	Sample description
ZP	Pure ZnO
ZP1	Zn _(0.99) O:P ₂ O ₅ (0.01)
ZP2	Zn _(0.985) O:P ₂ O ₅ (0.015)
ZP3	Zn _(0.980) O:P ₂ O ₅ (0.02)

The scanning electron microscopy is used to find out the morphological study. By using the XRD we can find out the phase analysis and crystal geometry. Fourier transform infrared analysis was carried out by using IR Prestige-21. With the help of Fluorescence Spectrophotometer the photoluminescence spectra of P₂O₅ doped ZnO were analysed. UV-Visible spectrophotometer is used to find out the band gap. Sample codes are enlisted in Table 1.

3.Results and Discussion

3.1 XRD Analysis

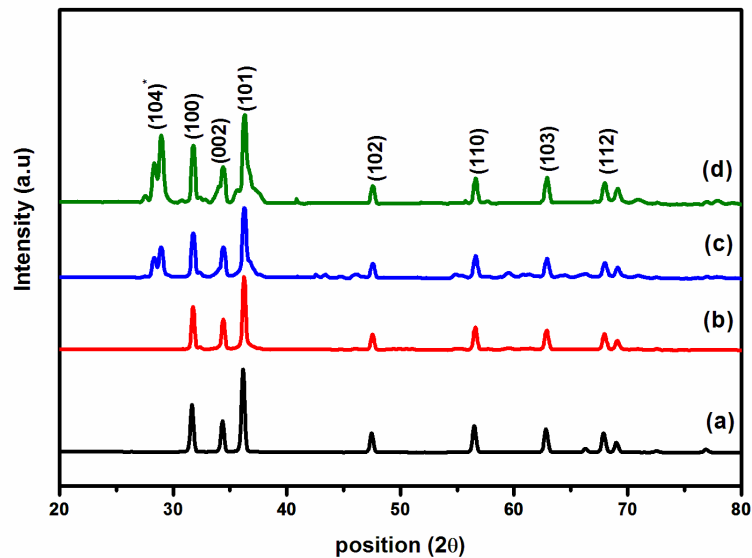


Figure 1. XRD patterns of a) ZP (b) ZP1(c) ZP2 (d) ZP3 nanophosphor

The XRD pattern obtained for P₂O₅ : ZnO NPs are recorded with 2θ ranging from 10° to 80° and it is represented in the Fig 1. The diffracted peaks at 2θ were assigned to lattice planes respectively in accordance with the JCPDS File No:87-0952 and 21-1486 respectively. It is observed that the P₂O₅: ZnO NPs possess hexagonal wurtzite structure. The crystallite size is evaluated using the Scherer Formula¹⁴:

$$D = \frac{K\lambda}{\beta \cos \theta} \quad (1)$$

Here K is the Scherrer's constant and its value is 0.9. λ is the wavelength of X-Rays, β is the full width of half maximum. From the Scherrer formula $P_2O_5:ZnO$ with three different concentrations having the crystallite size was calculated and is tabulated in Table 2. It can be seen that crystallite size varies with doping.

It is observed that XRD peaks originated from a crystal mainly due to various orientation of crystal planes. In which it comprises of many number of molecules exist in the form of unit cells which plays an important role.

Table 2. Crystallographic parameters of prepared samples

Sample details	'd' spacing (\AA)			Lattice parameters (\AA)			'Cell volume' V (\AA^3)	Crystallite Size 'D' (nm)
	100	002	101	a	c	c/a		
ZP	2.82	2.61	2.48	3.26	5.25	1.625	48.3183	29.6375
ZP1	2.83	2.60	2.48	3.28	5.18	1.568	47.4129	40.1298
ZP2	2.82	2.60	2.48	3.26	5.19	1.593	47.6741	44.1407
ZP3	2.82	2.65	2.48	3.26	5.18	1.594	48.2608	43.8129

3.2 FTIR Spectroscopy

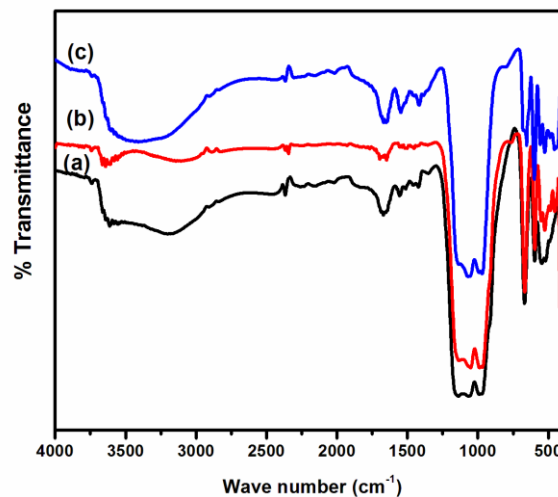


Figure 2. FTIR spectra of a) a) ZP1 (b) ZP2 (c) ZP3 nanophosphor.

By using the FTIR spectroscopy the composition, quality and molecular structure of the samples were carried out. It is observed that the FTIR spectrum of P_2O_5 NPs was recorded in the range of $400\text{--}4000\text{cm}^{-1}$. The characteristic absorption peak is in the region 958.5739 and 1099.51133 respectively and is given in the figure 3. The vibrational peaks at 400cm^{-1} to 500cm^{-1} indicates the presence of ZnO^{15-16} .

3.3. SEM Morphology

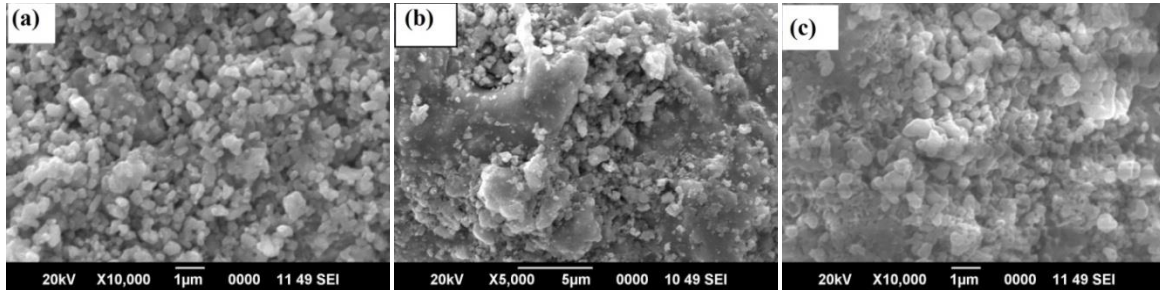


Figure 2. SEM image of a) ZP1, (b) ZP2 (c) ZP3 nanophosphor.

The SEM image of the P_2O_5 doped ZnO was recorded in the SEM operation mode. For electron production the filament voltage applied was 20kV with a magnification of 40000x. It is observed from the figure that it possesses spherical shaped structures. It is clear that the distribution of the particles present in the image was computed using image software. It is observed that the morphology is well ordered.

3.4. UV-Visible Spectroscopy

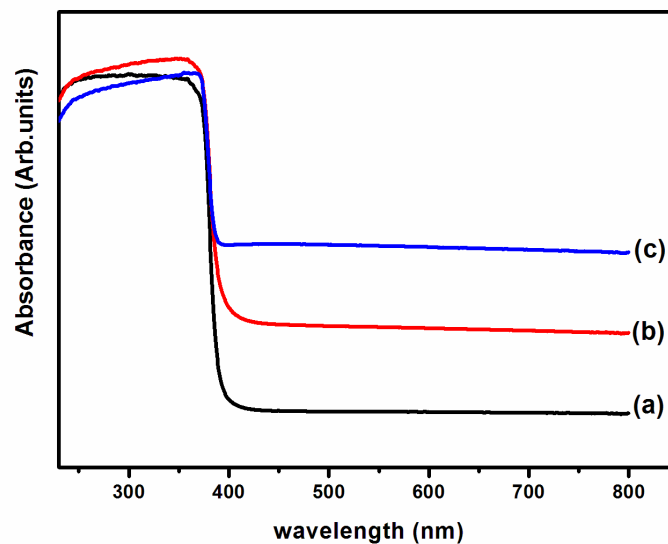


Figure 4. Absorbance spectra of a) ZP1, (b) ZP2 (c) ZP3 nanophosphor

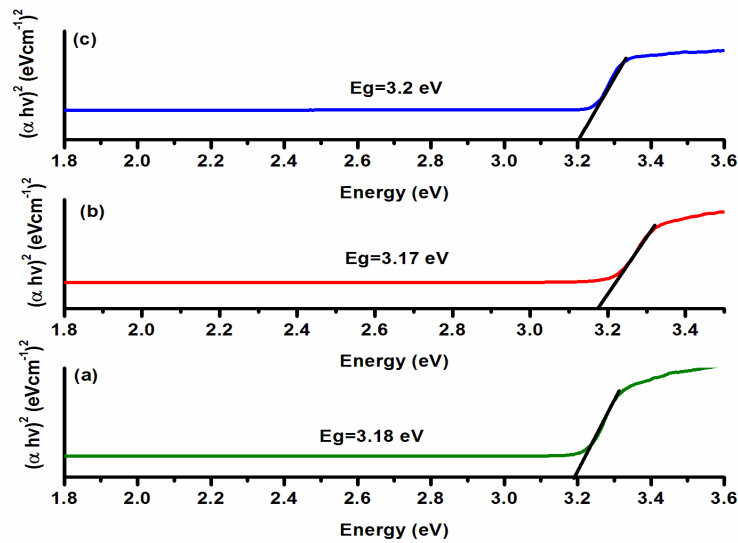


Figure 5. Tauc plot of a) ZP1 (b) ZP2 (c) ZP3 nanophosphor

The UV Visible spectroscopy of P_2O_5 : ZnO were taken in the solid state method. It is found that the absorption spectrum is a function of wavelength. The optical band gap values can be calculated by the following relation ¹⁷:

$$\alpha = A(h\nu - E_g)^n \quad (2)$$

where α is the absorption co-efficient, $h\nu$ the photon energy, A is a constant, and E_g is the optical band gap. 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.

By using Tauc plot we can find out the band gap. It is found that the band gap for ZP1, ZP2 and ZP3 are 3.18, 3.17 and 3.2 eV respectively. Due to quantum confinement, there is increase in the band gap, with the decrease in particle size and there is an optimum concentration in ZP2 sample.

Table 3. Band gap of prepared samples

Sample details	Bandgap (eV)
ZP1	3.18
ZP2	3.17
ZP3	3.2

3.5. Photoluminescence Spectroscopy

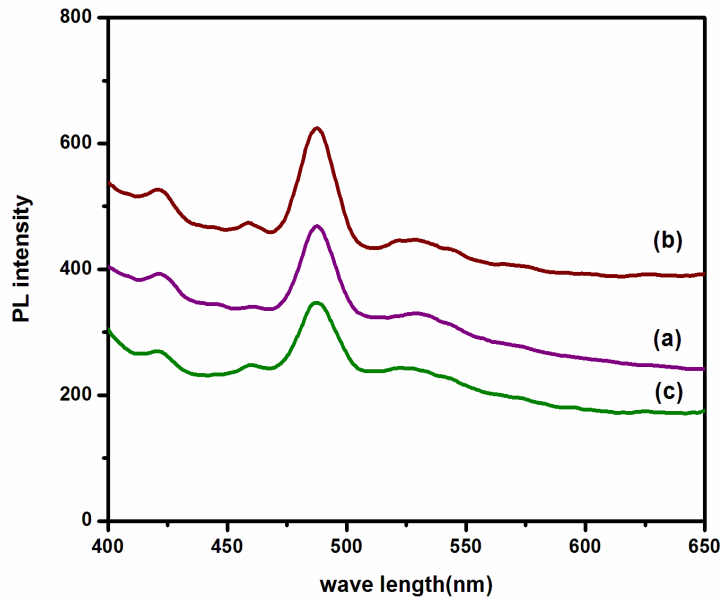


Figure 6. PL spectra of a) ZP1, (b) ZP2 (c)ZP3 nanophosphor

The photoluminescence spectrum of the $P_2O_5:ZnO$ were recorded in the solid state mode. The emission spectra of three different concentrations are shown in the figure with the excitation at 325nm. Most prominent emission of synthesized samples lies in the blue region, lower energy side corresponds to the deep level emission. Also a luminescence quenching effect can be observed in phosphor samples upto certain concentration. It is found that the origin of DLE is due to the oxygen interstitial defect found in the ZnO. The emission at 488 nm is due to the trap –state emission from $^5D_0 - ^7F_0$ ¹⁸⁻¹⁹.

4. Conclusion

The structure of the prepared sample was studied using X- ray powder diffraction pattern and FTIR. XRD pattern shows hexagonal wurtzite structure. The chemical groups of the sample were confirmed by the FTIR spectra. The SEM image of P_2O_5 doped ZnO micrograph revealed that the primary particles are uniform, circular in shape and weakly agglomerated. The UV Visible spectroscopic studies of the prepared samples were also carried out and the bandgap of the samples obtained are 3.18eV, 3.17eV and 3.2eV respectively. A blue luminescence quenching can be observed in samples upto an optimum concentration.

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