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Structural and Optical Properties of Znonanomaterial Using Co-Precipitation Route

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Abstract

Zinc oxide (ZnO) nanostructurematerial is synthesized via a co-precipitation method using chemical route for application in sensing devices, as functional additives in food packaging etc; The X-ray diffraction (XRD) analysis shows a pure phase formation of ZnOnano-powder. The estimated grain size is ~ 21 nm from XRD. Ultraviolet–visible spectroscopy and Fourier-transform infrared spectroscopy (FTIR) estimated the band gap of ZnO~ 3.3 eV and the presence of Zn-O-Zn vibration modes respectively. The growth of pure nano phase of ZnOopens up a simple way to synthesize ZnO nanoparticle for its utilization in novel functional devices.

1. Introduction

Among the many oxide material system[1],ZnO places its self at the top few oxide system which has been extensively studied in the last few decades due to its unique electronic and optical properties[2,3,4]. Recent technological development in the electronic and optical devices suggeststhat the thin film[5] of ZnO and nanostructures[6,7] have immense potential of becoming a promising candidate for development of novel electrical, optical and sensing devices. ZnO is found in abundant and is nontoxic with a direct band gap of

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3.4 eV. Due to wide band gap it lacks the absorption in the visible range hence restricts its application and performance as photocatalysts[8].The photoluminescence measurement suggests ZnO to have a large exciton binding energy of 60 meV. The estimated exciton bohr radius for the ZnOcalculated using belowequation is 1.4 – 3.5 nm.The higher exciton binding energy is essential for many novel optoelectronic devices.

$$a_b^* = \varepsilon_r(\frac{m}{\mu})\, a_b \qquad \text{---------- (1)}$$

Higher photo-stability, high electrochemical coupling coefficient, strong chemical stability and considerably large range of radiation absorptionmakes ZnO an even more intriguing multifunction materials to explore[8,9]. ZnO also possess piezo- and pyroelectric properties which can be utilized for sensing application, energy conversion devices and for photocatalytic hydrogen production[9**,**10,11**]**. On the other hand biodegradability, nontoxicity and biocompatibility makes ZnO a demanding materialin biomedicine application [9,12]. ZnO can exist in many structural form such as nano-rods, nanotubes, nano-spheres, nano-flowers etc;[13,14]. Usually high crystalline, good quality nanostructure films of ZnO nanostructures can be synthesized using gas phase form such as chemical vapor deposition, pulsed laser deposition and metal-organic chemical vapor deposition which requires high annealing temperature ranging from 450 – 900 °C[15,16,17].Contrary to that there are low temperature synthesis processes which are also utilized in order to prepare high quality ZnO nanostructure of different shape, size and morphology such as water solutionprecipitation, chemical solution and hydrothermal method.

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2. Sample Preparation Method

In this paper we report the growth and properties of nano-crystalline ZnO prepared through co-precipitation method using chemical route. Zinc nitrate hexahydrate [$Zn(NO_3)_2.6H_2O$, AR grade) (Merck), hexamethylenetetramine (HMTS) [$C_6H_{12}N_4$, AR grade] (Merck) were used as received. A solution of hexamethylenetetramine (HMTA) is mixed with $Zn(NO_3)_2.6H_2O$ and water in appropriate amount to have a final 0.1 M solution of 100 ml. The final solution was stirred at 60 °C for 30 min. The solution was then kept for precipitation for 24 hr. At the completion of the process the precipitate was washed by di water several time and final powder was then kept for calcination at 450 °C for 1 hr.

3. Results and Discussion

3.1Structural Characterization

Bulk structural characterization of ZnOnano-material was done using Bruker D8 discover powder X- ray diffraction.Figure 1 shows the X-ray diffraction over an angle between 20°-80° using Cu K_α radiation. These peaks matched with the zinc oxide (ZnO) hexagonal ICDD card number (79-0205). The observed peak at 2θ = 31.76°, 34.4°, 36.24°, 47.56°, 56.64°, 62.88°, 66.63°, 67.94° and 72.5° corresponds to (100), (002), (101), (102), (110), (103), (200), (112), (201), and (004) peak. The grain size (~21 nm) was estimated with the peak 2θ = 36.24° (101) having the highest intensity corrected for instrumental broadening. The calculated grain size was estimated using the Scherrer's formula.

$$g = \frac{0.94\lambda}{\beta_{eff}\,\mathrm{Cos}\theta} \qquad \text{---------- (2)}$$

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Where λ, wavelength (0.154 nm);θ, Bragg diffraction angle;β_{eff}, FWHM of the (101) diffraction peak of ZnO corrected for instrumental broadening. FULLPROF software was used to carry out the refine the XRD pattern. Pseudo-Voigt with axial divergence asymmetry function was used to model the diffraction peaks and linear interpolation was used to estimate the background (blue line). The estimated lattice parameter using rietveld refinement is, a (Å) = 3.248899, c (Å) = 5.203997, V ($Å^3$) = 47.57 for the ZnOnanomaterial.

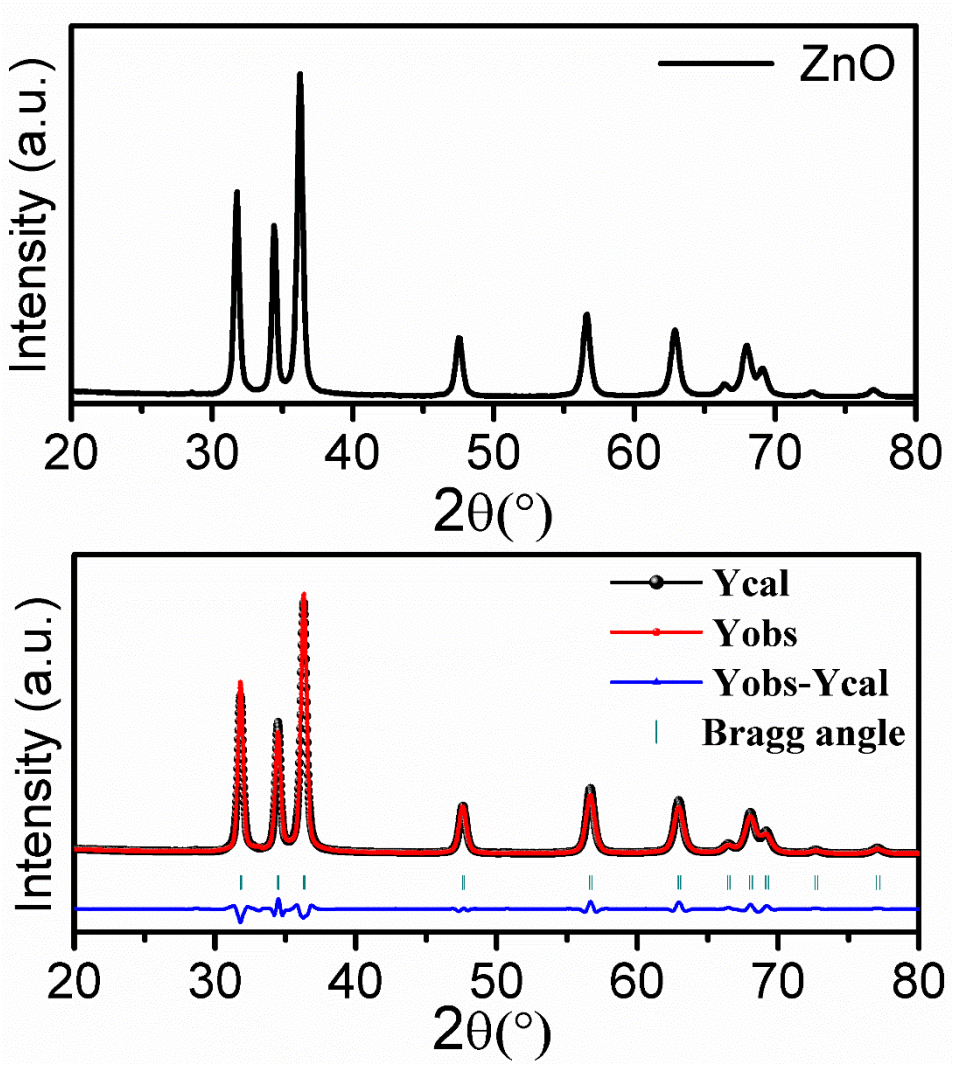

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Figure 1. X-ray diffraction of ZnO nanomaterial calcined at 450 °C in the 2θ range from 20° – 80°.

3.2FTIRMeasurement: ZnOwurtzite crystal structure, correspondence to $P6_3mc$ space group. It has 6 optical Raman modes $\Gamma = 1A_1 + 1E_1 + 2E_2 + 2B_1$ among which the $1A_1$ and $1E_1$ mode are both Raman as well as infrared active[18]. Fourier- transform infrared spectroscopy (FTIR) was done for the ZnO nanomaterial in the attenuated total reflection (ATR) mode using Perkin-Elmer Spectrum BX2 FTIR spectrometer. Figure 2 shows the transmittance spectrum in the range from 350 cm^{-1} to 1800 cm^{-1}. The strong absorption peak in 400 – 590 cm^{-1} range correspondence to Zn-O-Zn stretching modes and oxygen vacancy. The peak at 409 cm^{-1} correspondence to transverse (E_1) mode, ~ 426 cm^{-1}corresponds to Zn-O-Znstretching vibration modewhich is a characteristic of ZnOwurtzitestructure.

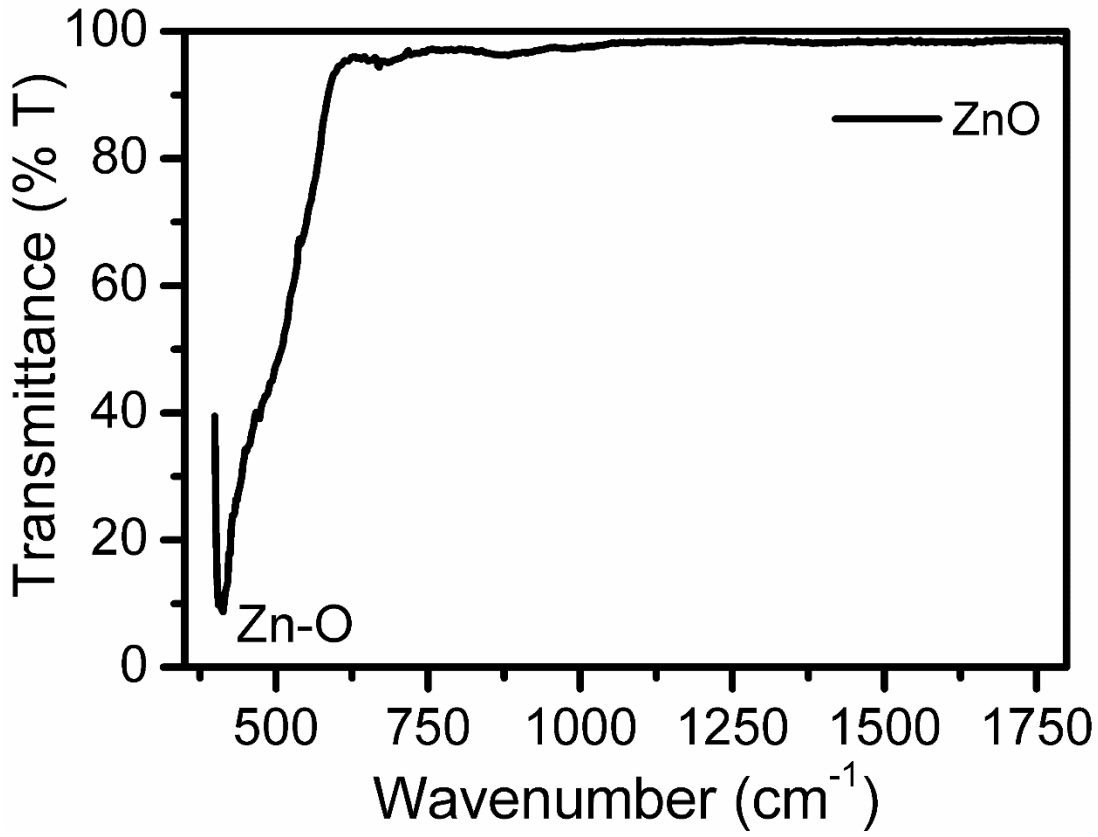

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Figure 2. Fourier- transform infrared spectroscopy (FTIR) of ZnO nanomaterial in the ATR mode calcined at 450 °C.

3.3Optical Band-Gap characterization: The band gap of ZnO nanoparticle depends on several parameters, such as; synthesis method, temperature, size, morphology and shape. Figure 3 shows the UV-Vis transmittance data of ZnO nanoparticle in the range from 1 eV to 4.0 eV. The band gap estimated using the Tauc equation from the UV-Vis data is ~ 3.45 eV which is comparable to the bulk values[19].

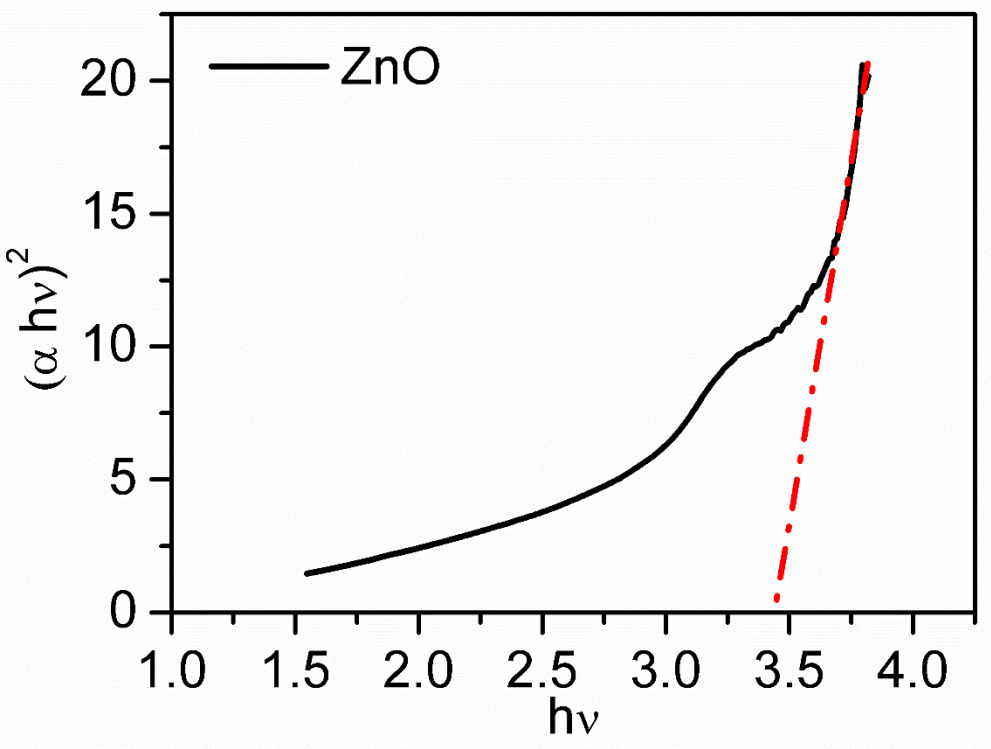

Figure 3.UV-Vis absorption data taken for ZnO nanomaterial calcined at 450 °C and $(\alpha h\nu)^2$ vs photon energy is plotted for optical band gap estimation.

4. Conclusion

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ZnO nanomaterial have been synthesized via co-precipitation route by stirring the zinc nitrate and HMTA solution and calcining the power at 450 ℃. The X-ray analysis confirms the pure phase formation of ZnO nanomaterials with average grain size ~ 21 nm. It is also corroborated by the presence of Zn-O-Zn stretching modes as seen in the FTIR transmission spectrum. The estimated band gap of ZnO nanomaterial synthesized by this route using UV-Vis spectrum is ~ 3.45 eV which is comparable to the bulk result. Hence these results suggests the pure phase formation of ZnO nanomaterials with relatively small grain size that have potential of being utilized for fabricating nano-sensing devices and as functional additives in food packaging.

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