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Structural and Optical properties of ZnO Nanoparticles

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Abstract

In this investigation, ZnO NPs were prepared through the co-precipitation method. ZnO NPs were characterized by X-ray diffraction (XRD), Field Emission Scanning Electron Microscopy (FESEM) and Energy dispersive analysis X-ray (EDAX). The different bond frequencies associated with the samples were assigned from their Fourier Transform Infra-Red (FTIR) spectra. The optical studies were explained by their UV-VIS and Photoluminescence spectra.

Keywords: ZnO NPs, XRD, FESEM, EDAX, FTIR, optical studies.

Introduction

The field of nanomaterials includes subfields that develop or study materials with unique properties that result from nanoscale dimensions. Surface science and colloidal science have created many materials useful for nanotechnology [1], such as carbon nanotubes and other fullerenes, various nanoparticles and nanorods. Nanoscale materials can also be used in large numbers of applications. Most of the current commercial applications of nanotechnology are in this flavor [2]. Advances have been made in using these materials for medical applications. See Nanomedicine. Nanoscale materials are sometimes used in solar

cells [3, 7], which is competing with the cost of traditional silicon solar cells. Development of applications containing semiconductor Display technology, lighting, solar cells, biological imaging like nanoparticles used in next-generation products [5]. Zinc oxide particles have been found to have superior UV blocking properties compared to their bulk alternatives [6, 8]. This is one of the reasons why it is commonly used in the production of sunscreen lotions and is completely light stable. This can be verified with higher glass transition temperatures and other mechanical property tests. These nanoparticles are hard and give them their properties.

Experimental and Characterization Methods

Synthesis

The following high purity chemicals such as Zinc (II) nitrate hexahydrate ($\text{Zn}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$), and Sodium hydroxide NaOH were used as the precursors without further purification. For the preparation of pure ZnO NPs, 0.1M of Zinc Nitrate hexahydrate was dissolved in 200ml of double distilled water and 0.8M of NaOH were separately dissolved in each 200 ml of double distilled water using two 200 ml beakers. Then, NaOH solution was added drop wise to the Zinc Nitrate solution which yields a white precipitate. The solution with the white precipitate was stirred at room temperature for 6 h. This solution was refluxed at room temperature for 24 h. Then, a clear solution was obtained, which found to be stable at ambient condition. Thereafter, the solution was washed several times with double distilled water and ethanol. Finally, the precipitate was dried at 120°C . Thus, ZnO nanopowder was obtained. Thus, sample was obtained. This sample was annealed at 700°C for 5 h because the energy from the heat could enhance the vibration and diffusion of lattice atoms crystallization.

Characterization Techniques

The ZnO NPs were characterized by X-ray diffractometer (model: X'PERT PRO PANalytical). The diffraction patterns were recorded in the range of 20° - 80° for the ZnO NPs sample where the monochromatic wavelength of 1.54 \AA was used. The sample was analyzed by Field Emission Scanning Electron Microscopy (Carl Zeiss Ultra 55 FESEM) with EDAX (model: Inca). The FT-IR spectra were recorded in the range of 400 - 4000 cm^{-1} by using Perkin-Elmer spectrometer. The absorption spectrum of ZnO NPs was studied in the range between 190 and 1100 nm by Lambda 36spectro photometer. Photoluminescence spectra were taken using spectrometer JASCO Spectro fluometer FP-8200.

Results and Discussion

X-ray diffraction Studies

The X-ray diffraction patterns of the prepared samples are shown in Fig. 1. The XRD peaks are located at angles (2θ) of 31.849, 34.508 and 36.334 corresponding to (100), (002) and (101) planes of the ZnO NPs. Similarly, other peaks found at angles (2θ) of 47.614, 56.668, 62.932, 66.45, 68.023, 69.106, 72.61 and 77 are corresponding to (102), (110), (103), (200), (112), (201), (004) and (202) planes of ZnO NPs. The standard diffraction peaks show the hexagonal wurtzite structure of ZnO NPs with space group $p63mc$. It is also confirmed by the JCPDS data (Card No: 36-1451).

This is the most stable phase of ZnO NPs. The lattice constants 'a' and 'c' of the wurtzite structure of ZnO can be calculated by using the relation [1],

$$\frac{1}{d^2} = \frac{4}{3} \left(\frac{h^2 + hk + k^2}{a^2} \right) + \frac{l^2}{c^2}$$

with the first order approximation ($n = 1$) for the (100) plane. The lattice constant 'a' is obtained through the relation $a = \frac{\lambda}{\sqrt{3} \sin\theta}$ and lattice constant

'c' is derived for the plane (002) by the relation $c = \frac{\lambda}{\sin\theta}$. The calculated values of 'a' and 'c' are

3.2418 \AA & 5.1941 \AA for ZnO NPs.

The average crystalline size of the samples is calculated by Debye Scherrer's relation

$$\text{Average crystalline size } D = \frac{k\lambda}{\beta D \cos\theta}$$

Where, λ - the wavelength of the radiation (1.54056 \AA for CuK radiation), k - a constant which is equal to 0.94, β - the peak width at half-maximum intensity, θ - the peak position. The average crystalline size is 33nm for ZnO NPs.

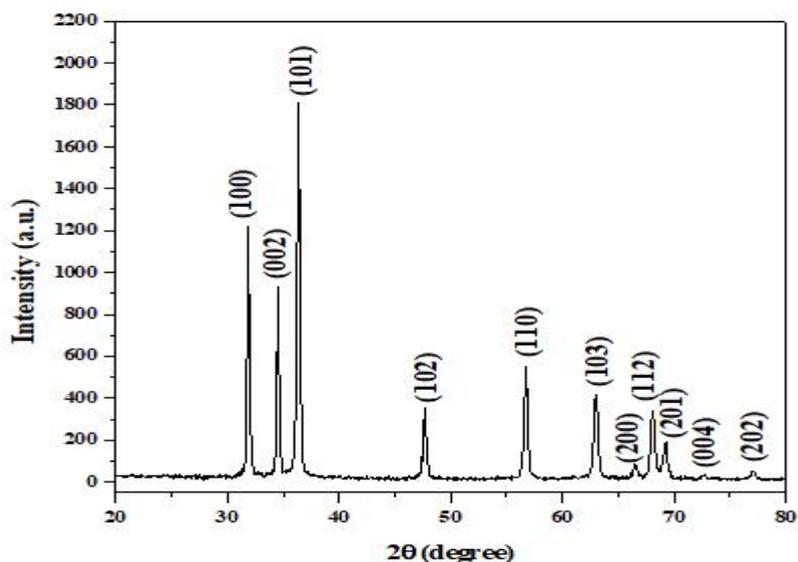


Figure 1. X-Ray Diffraction Pattern of ZnO NPs

Field Emission Scanning Electron Microscopic Studies

The FESEM is one of the promising techniques for the topography study of the sample and it gives important information regarding the growth mechanism, shape and size of the nanoparticles.

The surface morphology of the ZnO NPs is shown in Fig. 2 (a-b). The entire FESEM image clearly shows the average size of the NPs in the order of nanometer size. The ZnO NPs are tree like structure and top of tree uniform even grain boundaries formed. The uniform grain boundaries size 98 nm are found for the ZnO NPs.

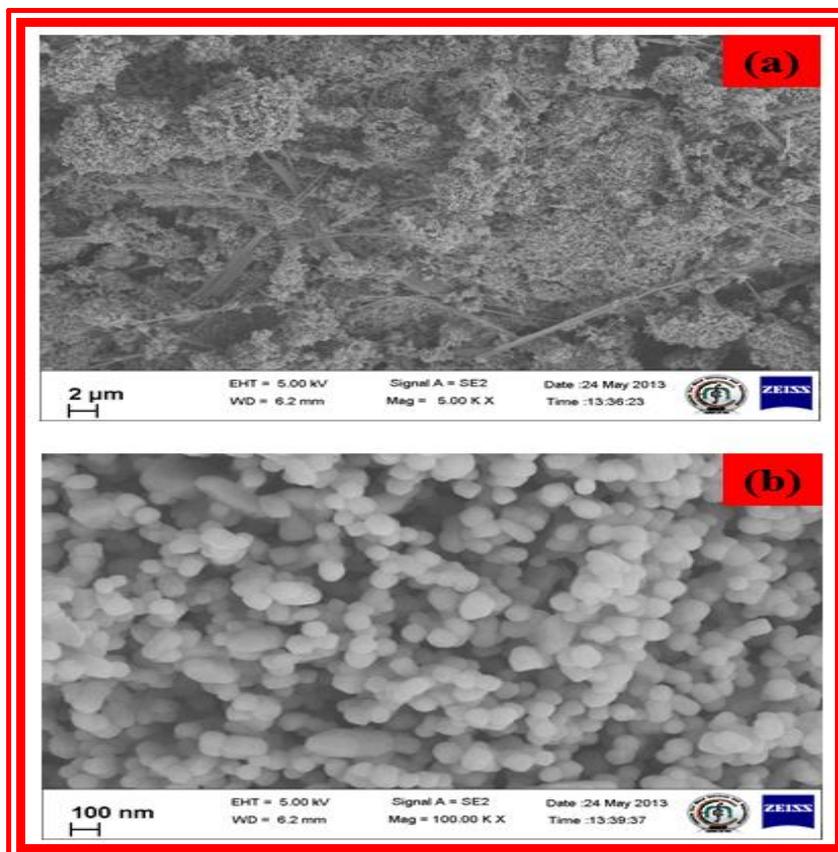


Figure 2. FESEM Image of ZnO NPs

Energy Dispersive Analysis X-Ray (EDAX) Spectra Studies

The chemical compositional analysis of ZnO NPs was carried out using EDAX. The typical EDAX

spectra of ZnO NPs are shown in Fig. 3. In the ZnO, the chemical composition of Zn and O are found as 51.61% and 48.39% respectively.

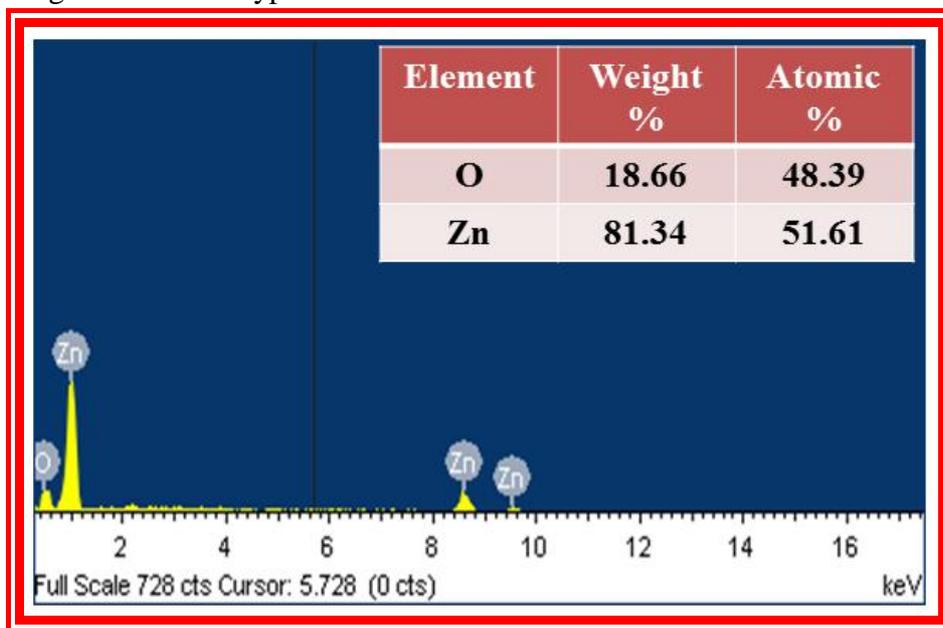


Figure 3. EDAX of Pure ZnO NPs

Fourier Transform Infra-Red (FT-IR) spectroscopic analysis

FT-IR spectroscopic analysis reveals the vibrational frequencies of the ZnO NPs. The recorded FT-IR spectra are shown in Fig. 4. The peak in the range of 3020-3650 cm^{-1} corresponds to the vibrational mode of O-H bonds [2]. The absorption peaks are observed at 3405 cm^{-1} for the ZnO NP sample due to the O-H stretching of

surface-absorbed water molecules. The asymmetric stretching vibration of C=O is observed at 1596 cm^{-1} ZnO NPs sample. The symmetric C=O bands are observed at 14436 cm^{-1} for the pure ZnO samples. The bands are observed at 876 cm^{-1} due to the C-H out-of-plane bending for the ZnO sample. The Zn-O stretching bands appear at 485 cm^{-1} for the ZnO NPs.

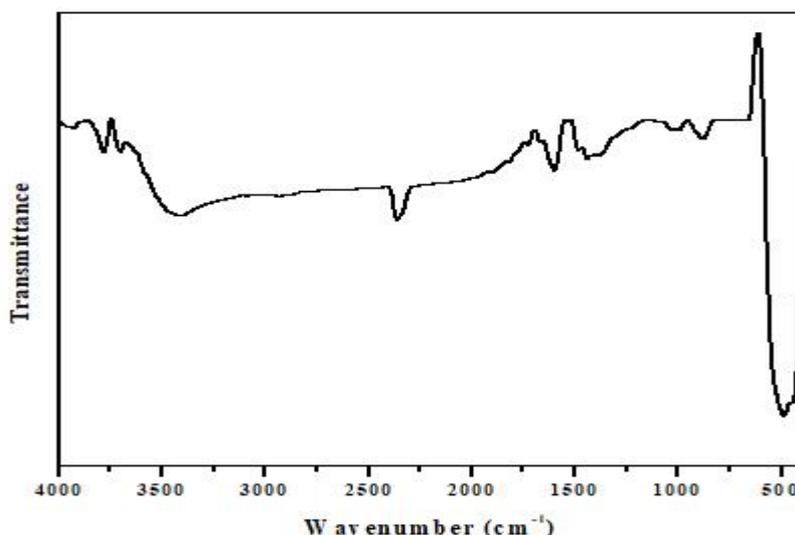


Figure 4 FTIR spectra of the ZnO NPs

UV-visible absorption spectroscopy studies

Figure 5 shows the UV-visible absorption spectrum ZnONPs. The ZnO samples absorption spectrum sharp peaks at 372 nm were observed, which believe to arise from the near band edge free excitons. The ZnO NPs are expected to show a small red-shift in comparison to bulk ZnO. The

band gap energies E_g , of ZnO NPs were found 3.3 eV. Showed the small 'red shift' of 0.07 eV from standard bulk band gap at room temperature ($E_g = 3.37$ eV). Where ZnO NPs result in decrease to deviating from the Burstein-Moss shift [3, 4] the estimated band gap values are close to the bulk ZnO, this gives conclusion that there is no indication of quantum size effect [5].

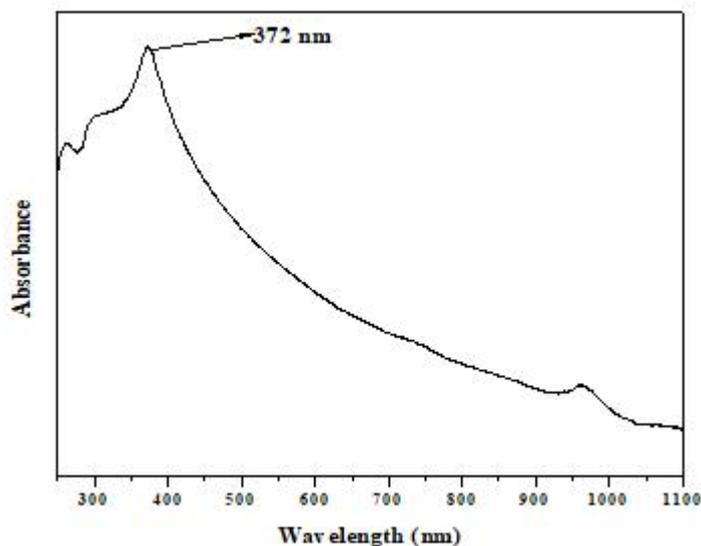


Figure 5. UV-visible spectra of ZnO NPs

Photoluminescence studies

The photoluminescence spectrum of the ZnONPs is shown in Fig. 6. The photoluminescence spectra of ZnO NPs samples recorded with the excited wavelength of 325 nm. The emission spectra of the ZnO NPs sample having six peaks at 395nm, 426nm, 440nm, 469nm, 483nm and 494nm. These bands are Near Band Edge emission, Violet emission, three blue emission and blue-green emission respectively. The NBE emissions is located at UV region 395nm for pure ZnO NPs, this NBE emission is attributed to the

radiative recombination between the electrons in the conduction band and the holes in the valence band. The violet emission centered at 426 nm, and is ascribed to an electron transition from a shallow donor level of the natural zinc interstitials to the top level of the valence band [5]. The three blue emission bands at 440 nm, 469 nm and 483 nm are attributed to singly ionized Zn vacancies [6]. There is blue-green emission band at 494 nm due to a surface defects in the ZnO NPs corresponding to the transition between oxygen vacancy and oxygen interstitial defect.

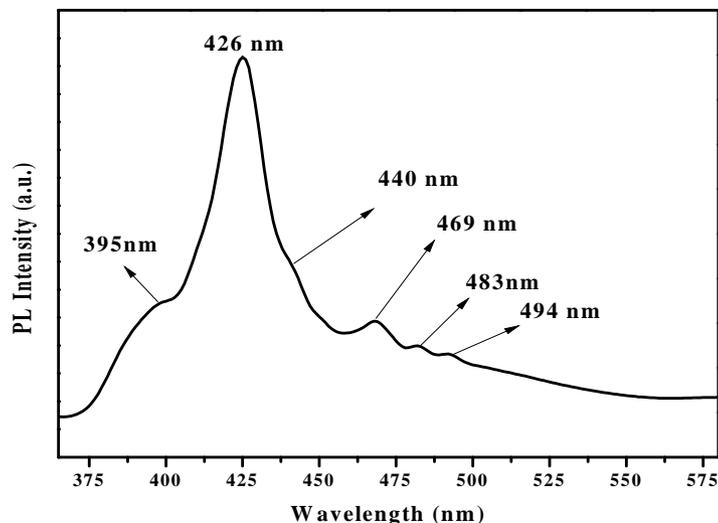


Figure 6. Photoluminescence emission spectra ZnO NPs

Conclusion

In summary, ZnO NPs was prepared through the co-precipitation method. The X-ray diffraction study confirmed that the prepared particles were in hexagonal wurtzite structure. The values of lattice parameters 'a' and 'c' were found to be 3.2418 Å & 5.1941 Å respectively for ZnO NPs. From the HRSEM images, the ZnO were tree like structure and top of tree uniform even grain boundaries formed. The uniform grain boundaries size 98 nm were found for the ZnO NPs. From the EDAX analysis, the chemical compositions were estimated. Using the recorded FT-IR spectra, the various vibrational frequencies were assigned for the ZnO NPs. From UV-Vis spectra, the ZnO sample absorption spectrum sharp peaks at 372 nm. The photoluminescence studies showed that the ZnO sample the band emission, which is due to zinc vacancies, oxygen vacancies and surface defects.

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