Synthesis and Characterization of Structural and Optical Properties of ZnO Nano-Particles

Madhuri Samel¹, Nileema Patil², Priya Tilak³

1LokmanyaTilak College of Engineering, Navi Mumbai, Maharashtra, India-400709

Abstract: In the recent era zinc oxide nanoparticles proved promising field for researchers due to their unique properties and applications in optoelectronic devices. (ZnO) is a distinctive electronic and photonic wurtzite n-type semiconductor with a wide direct band gap of 3.37 eV and a high exciton binding energy (60 meV) at room temperature. ZnO nanoparticles were prepared using wet chemical method with varying binder concentration of starch. Sizes of overnight dried suspension were determined using several analytical techniques. Theoretical and analytical considerations were evaluated, results were compared which confirms the formation of nanosize. Synthesized nanoparticles were characterized by XRD, AFM, particle size analyzer and UV visible spectrum etc. XRD AFM confirmed the nanosized zinc oxide particles. UV-spectroscopy shows the transparency of nanoparticles over entire visible range.

Keywords: Nano particles, sonication method, diffractometer

1. Introduction

ZnO nanoparticles have been famous among researchers as well promising candidate due to its various applications like gas sensors[1] bio sensors[2-3] solar cells[4] superconductors[5] varistors[6] photo detectors[7] photo catalyst[8], optoelectronic devices[9], cosmetics[10] etc. ZnO is distinctive electronic and photonic Wurtzite n-type semiconductor with a direct band gap of 3.37 eV and a high exciton binding energy (60 meV) at room temperature [11,12]. The high exciton binding energy of ZnO would allow for excitonic transitions even at room temperature, which could mean high radiative recombination efficiency for spontaneous emission as well as a lower threshold voltage for laser emission. The lack of a centre of symmetry in wurtzite, combined with a large electromechanical coupling, results in strong piezoelectric and pyroelectric properties and hence the use of ZnO in mechanical actuators and piezoelectric sensors [13, 14]. ZnO has high optical transparency and Luminescence in visible and near ultraviolet range of spectrum. Therefore, it is usually used in light emitting diodes and solar cells. ZnO nanoparticles are having high exciton binding energy nearly 60 meV. This means the excitonic transition in case of ZnO nanoparticles is possible at room temperature also [15-17]. Moreover many techniques are being used to synthesize ZnO nanoparticles Viz. precipitation method, spray pyrolysis method, micro emulsion method, hydro thermal method and Sol gel method. In the present investigation the sol-gel method for synthesis of ZnO nanoparticles was chosen as it is simplest method, consumes less power and can be carried out in robust atmosphere. Zinc Oxide is environmental friendly and ease to synthesize

2. Experimental Method

Zinc nitrate and sodium hydroxide are used as precursors. Starch has been used as stabilizing agent or binder. By using three different concentrations of stabilizing agent (0.1 %, 0.5 %, 1 %) three samples are prepared.

3. Structural Properties

During the present work X-ray diffraction pattern was recorded in 0-20 scan mode by using a JEOL JDX 8030 X-ray diffractometer at University department of physics, Santacruz, Mumbai. The radiation source used was Cu-Kα (λ=1.54018 Å). We have scanned the angle in the range of 20 to 80 degree. The Powder software was used to obtain data of XRD. Nanoparticle shows peak broadening. This broadening is observed for particles with diameter size less than 100 nm. In this case, particle size is measured by Debye Sherrer formula.

Particle size = 0.9 λ / FWHM (COS 0)

λ- the wavelength of the incident X-Ray
θ- is the angle corresponding to the peak FWHM- the full width at half maximum in radiance.

The comparison of the XRD s for the three samples is shown figure. It is seen that the peaks are obtained at same position but there is change in the intensities of respective peaks. The obtained peaks are comparable with the standard sample.

Average Particle size = 19.46 nm

Figure 1: Comparisons of XRDS

Figure 2: Temperature vs. Entropy

Figure 3: Temperature vs. Internal Energy
### 4. Comparison of Concentration with Particle Size

Table 1: Comparison of concentration with Particle Size

| Binder (conc.) | Particle Size (nm) |
|----------------|-------------------|
| 0.10%          | 19.46             |
| 0.50%          | 18.34             |
| 1%             | 17.08             |

For preparation of sample 1 we used 0.1% of starch as a binder in which we found average particle size as 19.46 nm. The 0.5% sample has average size of 18.34 nm and for 1% of starch sample average particle size reduced to 17.08 nm. It is seen from the above data that as the binder concentration increases the particle size goes on reducing. The experiment is carried out at room temperature.

Particle size = \(0.9 \lambda / \text{FWHM COS } \theta\)

Average Particle size = 19.46 nm

### 5. Morphological Study

The AFM imaging is carried out by using AFM machine by Vecco. The powder sample is sonicated in Distilled water. A drop of the dispersion is put on the glass. The surface is scanned by using the contact mode, which protects the surface damage. The 3D images of samples are given above. It is seen that particle are not separate out but agglomeration is observed. We tried different techniques of sample preparation for imaging purpose but could not get the well-separated particles. The particle size varies from 30 to 100 nm. There may be cluster formation.

### 6. Optical Properties

The UV spectra obtained by using SHIMADZU UV-2401 machine at university department of chemistry for the various samples in shown below. The incident in wavelength is in the range of 300 – 800 nm. The sample will be absorbing wavelength depending on its concentration. The sample was prepared by sonication method. The small quantity of the powder sample was added to the distilled water. This solution was sonicated to get dispersion of the sample. Then this dispersion was pour in the reference cell for UV Absorption. The size of the nanoparticles is crucial factor to determine properties of materials. Thus, size evolution of semiconducting nanoparticles becomes very essential to explore the properties of the materials. UV-visible absorption spectroscopy is widely being used technique to examine the optical properties of nanosized particles. The absorption spectrum of ZnO nanopowder is shown in Figure. It exhibits a strong absorption band at about 355 nm an excitonic measurement.

Band Gap is calculated by using following formula-

\[ E_g = \frac{hc}{\lambda} \]

For sample 1 (0.1% starch)

\[ \lambda = 360 \text{ nm} \]

\[ E_g = 3.47 \text{ ev} \]

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**Figure 2:** 3D AFM image of sample

**Figure 3:** 3D image of Sample

**Figure 4:** Absorption Spectra

| Binder concentration | Absorption coefficient | Exition Wavelength(nm) | Band Gap(ev) |
|----------------------|-----------------------|------------------------|--------------|
| 0.1                  | 1.663                 | 360                    | 3.47         |
| 0.5                  | 1.729                 | 360.5                  | 3.46         |
| 1                    | 0.54                  | 372.5                  | 3.35         |
Using Following equations

\[ 3.8 \frac{R^2}{R} = \left( \frac{n-1}{n+1} \right) \]

R - Reflectance coefficient.

n - Refractive Index

From the reflectance spectra of the Zno at wavelength 250 the coefficient is 1.2 % i.e

R = 0.12

Substituting in the above equation it gives

n = 1.0292

The optical density is given by

ln(1-R)² / T

Optical density = 0.275

7. Results and Discussion

ZnO nanoparticles have been prepared using wet chemical synthesis method and were characterized by XRD, AFM ,UV-vis absorption,. XRD and AFM studies confirmed the nanostructures for the prepared ZnO nanoparticles. The Absorption spectra gives the band gap value. The excitonic wavelength goes on increasing as the binder concentration increases. The value of Band gap goes on decreasing as per increasing binder concentration. The reflectance spectra show that at the excitonic peak in absorption spectra dip is observed in the Reflectance spectra. The prepared ZnO nanoparticles exhibit (λ exc = 360 nm) sharp UV band corresponding to near band gap excitonic emission at room temperature. These ZnO nanoparticles can be used in different industrial applications, namely, luminescent material for fluorescent tubes, active medium for lasers, sensors, and so forth.

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Author Profile

Mrs. Madhuri Samel is having M.Phil. and M.Sc. degree in Physics. Currently she is working as Assistant Professor in Applied Physics department at Lokmanya Tilak College of Engineering; Navi Mumbai.

She is having total teaching experience of 8 years.
**Mrs Nileema Patil** is having M.Sc. degree in Physics. Currently she is working as Assistant Professor in Applied Physics department at Lokmanya Tilak College of Engineering; Navi Mumbai. She is having total teaching experience of 12 Years.

**Mrs Priya Tilak** is having M.Sc. degree in Physics. Currently she is working as Assistant Professor in Applied Physics department at Lokmanya Tilak College of Engineering; Navi Mumbai. She is having total teaching experience of 19 years.