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Structural and Photoluminescence Properties of ZnO Nanoparticles Prepared by Solution Combustion Method

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Abstract— *This paper reports on the structural and photoluminescence properties of ZnO nanoparticles prepared by solution combustion method, using zinc nitrate and sugar. X-ray diffractometer SEM, EDAX, Raman spectroscope, Fourier transform infrared (FTIR) and photoluminescence (PL) spectrophotometers were employed to study the structural and optical properties. The XRD results indicated that the synthesized ZnO nanoparticles had pure wurtzite structure. Size of the nanoparticles was determined using Scherer's formula. The SEM gives the agglomerated fluffy nature of ZnO. FTIR confirms the characteristic vibrational mode of ZnO bonding at 417 nm. ZnO exhibits a direct band gap of 3.37eV at room temperature with a large exciton energy of 60 meV.As a result ZnO is recognized as a promising photonic material in the blue ultraviolet region. Photoluminescence behavior of the prepared sample shows a strong UV emission at 395 nm, violet emission at 405 nm and blue band emission at 480 nm.Weak band around 520nm in the green region are also recorded*

Keywords— *ZnO, Photoluminescence, XRD, SEM*

PACS Code— *60*

1. INTRODUCTION

Zinc oxide (ZnO) is a wide band gap semiconductor with wurtzite structure. The physical and chemical properties of nano-scale particles are different when compared with the bulk materials. Nano powders controlled to nanocrystalline size can show atom like behavior which results from higher surface energy. It is due to the large surface area and wider band gap between the conduction and valence band [1].There is a need for the improvement of the synthesis of ZnO for less time and less expensive. Alternate method was proposed by various people Park *et al.* proposed and reported a novel solution combustion method (SCM) [2]. ZnO nanoparticles are used in a variety of applications such as UV absorption, antibacterial treatment, UV light emitters, photocatalyst and as an additive in many industrial products [3]. It is also used in the fabrication of solar cells, gas sensors, luminescent materials, transparent conductor, heat mirrors and coatings.

2. EXPERIMENTAL

In the actual synthesis zinc nitrate (5g) and sugar (1.2g) are dissolved in a minimum quantity of water in a cylindrical pyrex dish of 300ml capacity and stirred well for half an hour. The redox mixture is rapidly heated in a muffle furnace at 300°c with a flame temperature of 1000°c and thermally dehydrate forming a honey like gel which ignites to give voluminous zinc oxide powder. The muffle furnace operates on 240 volts AC, 13.75 Amps current..It has power rating of 3.3 KW and an operating volume of 35 x 15 x 15 cm^3.The average heating rate was 10°C per minute. Cr-Al thermocouple was used to measure the furnace temperature.

The theoretical equation can be written as,

$Zn(NO_3)_2+C_{12}H_{22}O_{11}\rightarrow ZnO+N_2+11H_2O+12CO_2$

3. RESULTS AND DISCUSSION

The powder X- ray diffraction patterns of ZnO nano particle synthesized by solution combustion method is shown in Figure 1.

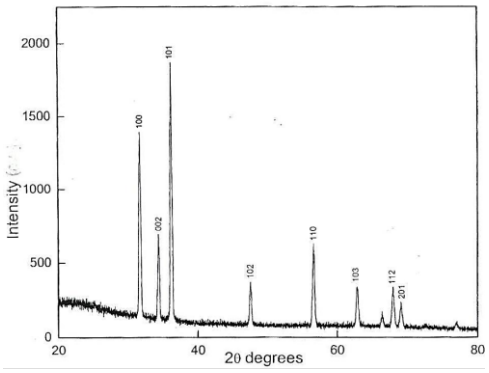

Fig. 1: XRD pattern of ZnO Nanoparticle

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The X-ray diffractometer was used to confirm the crystalline phase of ZnO powder. The peaks at 2θ = 31.67°, 34.31°, 36.14°, 47.40°, 56.52°, 62.73°, 67.91°and 69.03° were assigned to (100), (002), (101), (102), (110), (103), (112) and (201) of ZnO NPs indicating that the samples were polycrystalline wurtzite structure. The particle size D of ZnO was estimated from the Full Width Half Maximum (FWHM) of the diffraction of the powder, using Sherrer's formula.

$D=K\lambda/\beta_{½}\cos\theta$.

Where λ is the wavelength of X-ray, θ is the Bragg angle and K is a constant depend on the grain shape. $\beta_{½}$ is the FWHM. XRD studies are carried out using a Philips powder X –ray Diffractometer (model pw 1071) with Ni filtered Cu-Kα radiation. The average size of the ZnO nanoparticle is in the range of 48 nm.. All the diffraction peak in the pattern can be indexed as the pure hexagonal shape of ZnO with space group p63mc. This indicates that the sample is composed of wurtzite structure of ZnO, with the lattice points a=3.249 and c=5.206 °A which are consistent with the values in the standard card.(JCPDS 36-1451).Compared to the standard card the (002) peak is stronger, revealing the (001) oriented growth of the ZnO nano/microparticles[4].

Figure2 shows the SEM picture of ZnO powder. The porous, agglomerated fluffy nature with micro rods of the ZnO powder is recorded. The porous and voids are due to a lot of gaseous products generated during combustion.

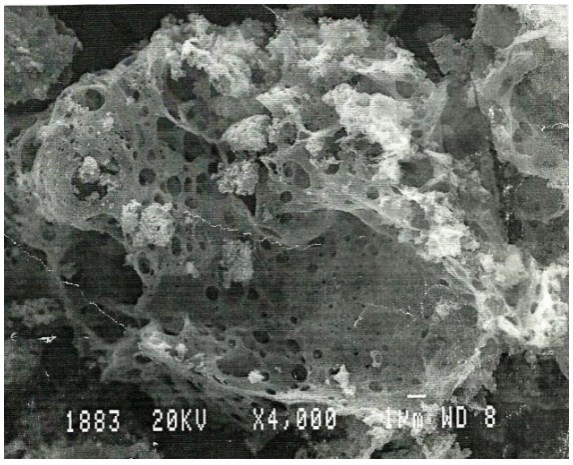

Fig. 2: SEM picture of ZnO prepared by solution combustion method

The average composition of the sample was obtained from EDS spectra recorded at different areas are shown in Figure3. The position of the peaks give information about the atomic specious, while peak areas provide information about the amounts of each atom present in the sample The X-ray lines of oxygen occur close to the detection limit of EDS detector. So the analysis does not provide information about oxygen

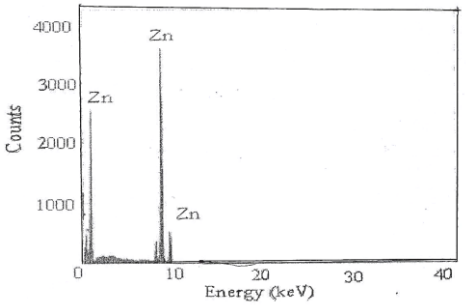

Fig. 3: EDAX spectra of ZnO nanoparticle

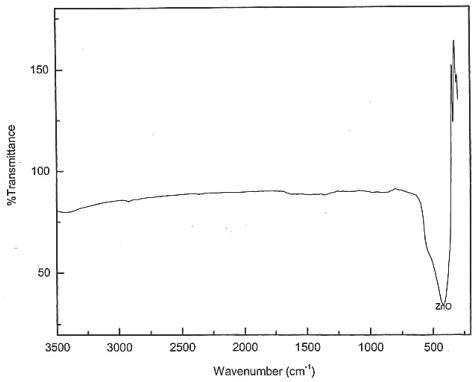

Fig. 4: FTIR spectrum of ZnO.

FTIR studies are carried out using Perkin-Elmer 1000. for as-prepared samples. FTIR spectra are recorded using thin pellets of the samples made with KBr. Figure 4 shows the FTIR spectrum in the range of 4000-330 cm^{-1} nano ZnO powder. There is only one significant band at around 417cm^{-1} associated with the characteristic vibrational mode of ZnO bonding [5].The absorption peak at 3421 cm^{-1} corresponds to the-OH group of water absorbed on the surface of the ZnO powder.

Raman spectroscopy was carried out to study the vibrational properties of as- prepared ZnO.is shown in Figure 5.

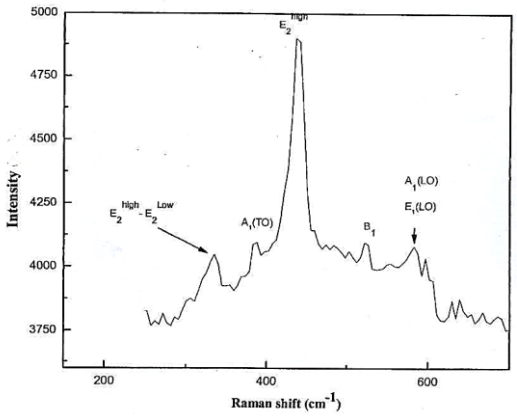

Fig. 5: Raman scattering spectrum of ZnO

The Raman peaks at 384 and 407 cm^{-1} came from A1 (TO) E1 mode of ZnO respectively. The strong peak at 438cm^{-1} and weak peak at 334cm^{-1}, which are assigned to theE2 and 2E2 modes which are a typical Raman active branch of hexagonal ZnO [6]. The peak at 532cm^{-1} is broadened which indicates that it may be a compound mode mixed with A1 (LO) and surface modes [7].

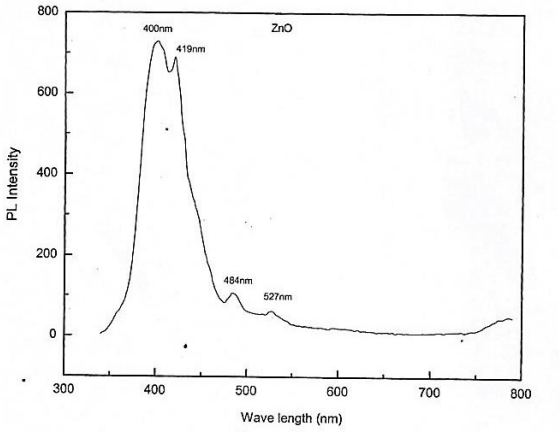

Fig. 6: Photoluminescence spectrum of ZnO NPs

Figure 6 shows the PL spectrum of ZnO nanopowder with particle size 48nm.It shows strong UV emission at 395 nm and violet emission at 405 nm.The emission in the UV region is attributed to the recombination between electrons in the conduction band and holes in the valence band [8].Violet emission at 405 nm is attributed to the exciton transition [9].The strong UV emission and weak green emission in PL spectra indicate that the ZnO particles have a good optical quality with few oxygen vacancies [10].In addition to the peak discussed above it shows blue emission at 484nm and green emission at 527 nm. Blue emission at 484 nm is electron transition from the shallow donor level of Zn interstitials to the valence band. The weak green band emission corresponds to the singly ionized oxygen vacancy in ZnO and this emission results from the recombination of a photo generated hole with the singly ionized charge of the specific defect [11].Oxygen vacancies are considered as the most common defects and considered as radiative centers in luminescence process. So the single crystalline ZnO nanoparticles are promising as a high performance optical material [12].

4. CONCLUSION

In this study nano sized ZnO powder was synthesized using the solution combustion process and the results leads to the following conclusion.

Powdered XRD confirms the crystallinity of the ZnO sample. Particle size is determined by Scherer's formula and found to be 48nm.The SEM gives the agglomerated, fluffy nature with micro rods are recorded. FTIR confirms the characteristic vibrational mode of ZnO bonding at around 417nm. The Raman peaks at 384 and 407cm^{-1} came from the A1(TO) and E1 mode of ZnO respectively. The strong peaks at 438cm^{-1} and a weak peak at 334 cm^{-1}, which are assigned to the E2 and 2E2 modes which are a typical Raman active branch of hexagonal ZnO. The excellent room temperature UV emission property should be attributed to the high purity and perfect crystallinity of the synthesized ZnO nanoparticles. Strong UV emission at 395nm, violent emission at 405nm and blue band emission at 484nm are recorded. Weak band around 520nm in the green region also is recorded.

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