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Insights into Structural and Optical Properties of ZnO Nanoparticles

Gunjan E. Yenorkar[1], Lukesh D. Giradkar[2], Arpit D. Wagh[3], S. T. Bahade[4]
[1, 2, 3]*Department of Physics, Nabira Mahavidyalaya, Katol, India*
[4]*Department of Electronics, Nabira Mahavidyalaya, Katol, India*

Abstract: ***ZnO nanoparticles have been synthesized from zinc nitrate as precursor and potassium hydroxide as precipitating agent using precipitation method. The prepared nanoparticles were characterized by using X-ray diffraction, Fourier Transform Infrared Spectroscopy (FTIR) and UV-Visible Spectroscopy analysis confirmed the formation of ZnO nanoparticles having hexagonal unit cell and wurtzite structure. The FTIR analysis provided information about the presence of functional groups in prepared nanoparticles. The UV-Vis absorption spectrum showed prominent peaks near to 360nm range whereas small peaks were also seen near to that region. The energy band gap and Urbach energies were also calculated as 3.16ev and 0.11364ev using Tauc plot and Urbach energy plots respectively. The synthesis method demonstrated simplicity and scalability, suggesting its potential for large-scale production in various applications.***

Keywords: ZnO Nanoparticles, precipitation, Tauc Plot, Urbach energy

I. INTRODUCTION

Recent researches in the area of nanotechnology are to prepare properly and highly ordered small nanoparticles[1]. This nanoparticle employs application in various fields of science and technology. Nanoparticles due to their high surface to volume ratio differs in their electronic, optical, morphological, structural and many more properties from their bulk states. The variation of this properties has led to formation of nanoparticles for various applications. ZnO being one such material has gained significant interest due to its distinct nature of being n-type semiconductor with wide and direct energy band gap of nearly 3.37ev and high excitations energy of nearly 60meV at room temperature[2]. Basically, ZnO is white odorless solid having molecular weight of 81.36gm/mole with wurtzite crystal structure. Refractive index of nearly 2.0041 is seen whereas density is found to be 5.606gm/cm^3 with melting point of $1975^o c$. ZnO have two crystal structures hexagonal wurtzite and cubic zinc blende. Wurtzite being more stable is prepared mostly in environmental conditions[3]. ZnO possess excellent chemical stability and due to different chemical and physical properties arising due to dependency on morphology of structure various techniques such as solgel method, microemulsion, spray pyrolysis, ultrasonic, microwave, chemical vapor deposition, hydrothermal and precipitation methods have been employed for preparation ZnO nanoparticles[4][5][6][7]. ZnO have found remarkable applications in semiconductor devices, piezoelectric sensors, gas sensors, luminescent materials, magnetic materials, catalyst and so on. As ZnO has high thermal conductivity, high binding energy, high refractive index it is used in medicine, solar cells, rubbers and as antibacterial in foods as well

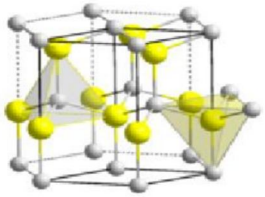

Fig. (1): Wurtzite unit cell

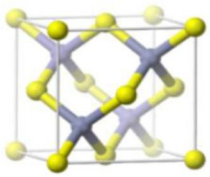

Fig (2): Zinc blende unit cell

II. SYNTHESIS

In this work ZnO nanoparticle have been prepared using co-precipitation method. (0.4) M of 1.122gm Potassium hydroxide was added to a beaker containing 50 ml of distilled water. In another beaker 0.2 M of 2.97gm of zinc nitrate was added to 50 ml of distilled water. Both the solution was mixed and stirred for 2 hours continuously. This continuous stirring resulted in the formation of white suspension which represented formation of ZnO Nano particles in precipitate form. The obtained precipitate was washed s firstly with 100% alcohol once and followed by distilled water three times. The product was then filtered using filter paper and were dried for 3 hours at 200°.C This dried sample were then finely crushed in mortal pester to obtain ZnO Nanoparticles.

III. RESULTS AND DISCUSSION

A. *X-ray Diffraction*

Figure (3) represents the XRD pattern of prepared ZnO nanoparticles. The broadening of peaks and definite lines represents material having particle in different range of nanoscale. The peaks were found to be located at $31.74^o, 34.39^o, 36.22^o, 47.49^o, 56.54^o, 62.79^o, 67.96^o, and\ 69.02^o$ corresponding to (100),(002),(101),(102),(110),(103),(112) and (201) (hkl) planes respectively. The peaks of prepared samples located at different (2θ) were found to closer to standard xrd peaks of ZnO nanoparticles JCPDS data. The comparative of prepared and standard ZnO nanoparticles data is given in table no (1) below. Maximum intensity peak was obtained at 36.22^o corresponding to (101) plane. The complete data obtained with values of lattice constant a=b=3.25A^o and c=5.21A^o and lattice parameter as α=β=90^o $and\ \gamma = 120^o$ gave confirmation about hexagonal unit cell and wurtzite structure. Diameter of ZnO nanoparticles was calculated by using Debye-Scherer formula $D = \frac{0.89\,\lambda}{\beta cos\,\theta}$

where 0.89 = Scherrer constant

λ= wavelength of X-ray

β=Full Width at Half Maximum (FWHM)

The diameter was found to be 48.14 nm corresponding to maximum intense peak located at 36.22^o

Table No :1

(hkl) plane	JCPDS (2θ)	Prepared Nanoparticles(2θ)
100	31.76	31.47
002	34.42	34.39
101	36.25	36.22
102	47.53	47.49
110	56.60	56.54
103	62.86	62.79
112	67.69	67.96
201	69.09	69.02

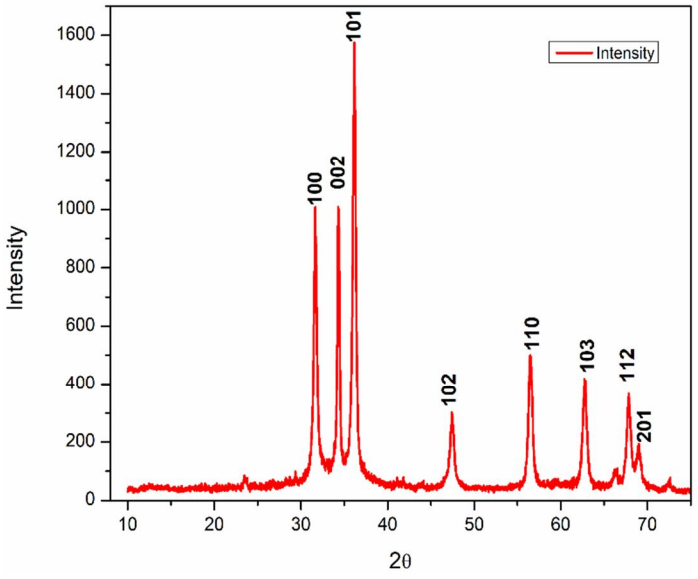

Fig (3): XRD of ZnO Nanoparticles

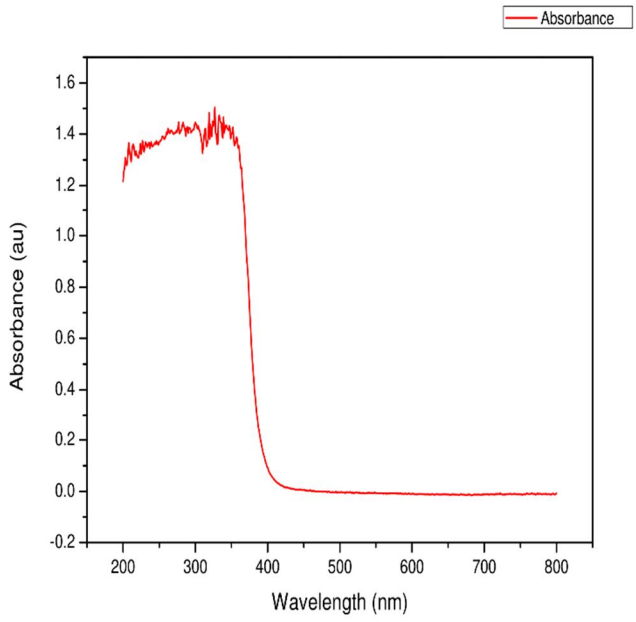

Fig (4): Absorption Spectrum of ZnO Nanoparticles

B. Absorption Spectrum

In the study of ZnO nanoparticles, the absorbance spectrum was analyzed within a range of 200nm to 800nm. Notably, peaks were observed around 360nm, a characteristic feature of ZnO nanoparticles, confirming their formation. Additionally, there were some additional peaks in proximity to this wavelength, suggesting possible impurities or defects in the nanoparticles. The band gap of the ZnO nanoparticles was determined to be 3.16eV. This determination was made by plotting a graph between the square of the absorption coefficient (α) multiplied by the photon energy (he) and the energy of the photons in electron volts (eV). Extrapolation of this graph allowed for the identification of the band gap energy. Furthermore, the Urbach energy of the ZnO nanoparticles was calculated to be 0.1134eV. It was done by plotting a graph between the natural logarithm of the absorption coefficient (ln(α)) and the energy of the photons in electron volts (eV), with the Urbach energy being the inverse of the slope of this graph

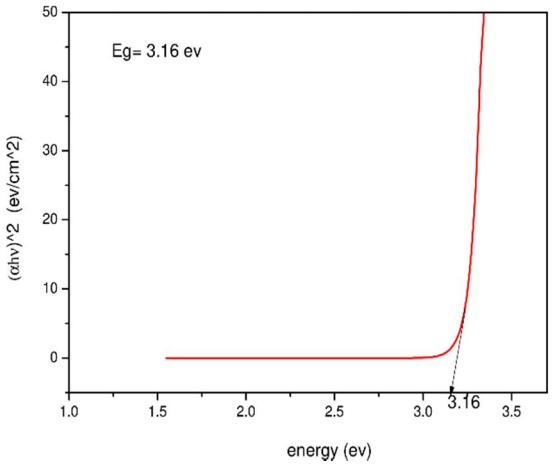

Fig (5): Tauc Plot

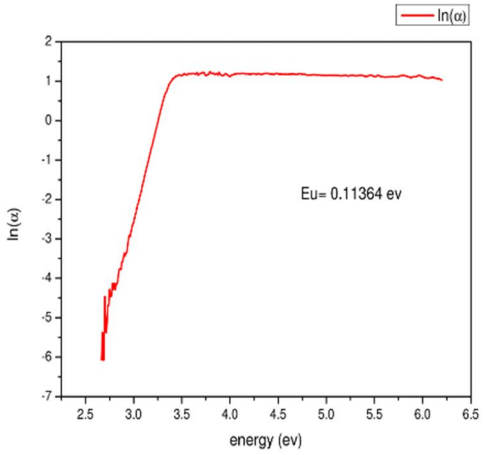

Fig (6): Urbach Energy Plot

C. Fourier Transform Infrared Spectroscopy (FTIR)

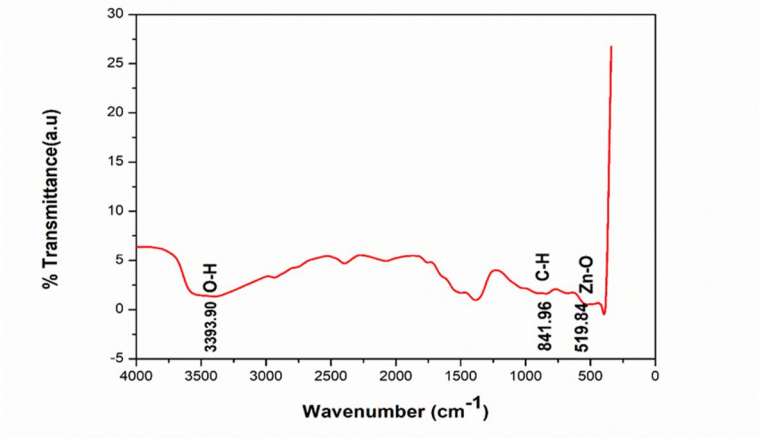

Fig. (7): FTIR of ZnO Nanoparticles

FTIR spectra of ZnO nanoparticle was recorded in the range of 4500-500 $cm^{-1.}$ IR spectra shows absorption peak around 3393.90 cm^{-1} which shows OH stretching vibration. The strong peak around 519.84 $cm^{-1}$is shows stretching vibration of Zn-O bonds. The peak around 841.96 cm^{-1}shows vibration of C-H bond

IV. CONCLUSION

In the present work, zinc nitrate and KOH precursors were used to synthesize ZnO nanoparticle by co- precipitation method. The particles were then analyzed using XRD, FTIR, and-UV-VIS optical absorption spectroscopy XRD verified the development of ZnO's wurtzite structure which has crystalline size of 48.14 nm corresponding to maximum peak at 36.22^{o}. The FTIR spectra provided additional confirmation of the structural characteristics of nanoparticles and confirmation of ZnO Nanoparticles.

FTIR spectra were also used to predict different functional groups showing prominent peak at 519.84 cm^{-1}. From UV-Visible spectra absorption peak was obtained around 360nm whereas energy band gap and Urbach energies were also calculated as 3.16ev and 0.11364ev respectively. According to the result, the manufacturing procedure used in this work was straightforward and inexpensive.

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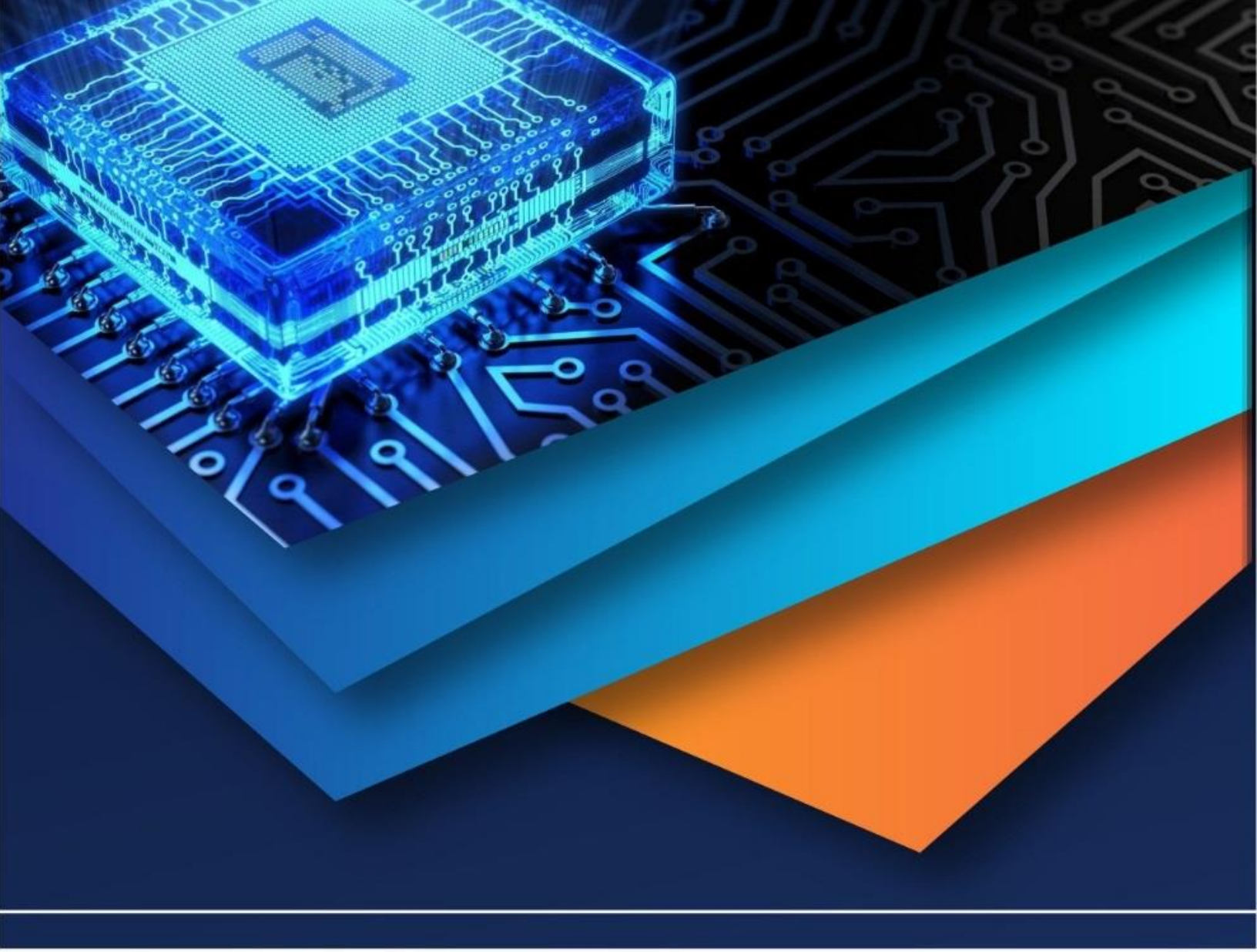

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