International Journal of Scientific Research in Physics and Applied Sciences
Research Paper Vol-3, Issue-1 E-ISSN: 2348–3423

X-Ray Diffraction Study of ZnO Nanoparticles

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Abstract- Zinc Oxide (ZnO) is the most versatile material as it has high mechanical & thermal stability. It has a wide band gap of 3.5 eV which gives this material various properties such as optical and physical property. It is used in different applications such as in electronic devices, sensors, biomedical fields etc. In our work ZnO nanoparticles were synthesized using chemical precipitation method. The ZnO nanoparticles were characterized using X-ray Diffraction (XRD) techniques by Scherrer formula & theoretical characterization done by effective mass approximation method. The particle size is estimated and compared by both practical & theoretical method. Both the results obtained by practical and theoretical methods are found to be in a good agreement.

***Keywords**:* ZnO nanoparticle,XRD

1. INTRODUCTION

Semiconductor nanomaterials have received great attention due to its wide band-gap. Among these various semiconductor oxide nanomaterials zinc oxide is a versatile material because of its physical-chemical properties such as mechanical, electrical, optical, magnetic and chemical sensing properties. It has a wide band gap of 3.5 eV. It is used in various applications like uv light emitters, spin functional devices, gas sensors, transparent electronics and surface acoustic wave devices, biomedical field. ZnO also has industrial applications such as cosmatics, pharmaceuticals, plastics, rubber, soap, textile, batteries etc.

Different types of synthesis techniques are used for the synthesis of Zno nanomaterials such as bottom-up approach; viz sol-gel technique,chemical precipitation technique and in top-down ; ball milling etc. The precipitation technique gives high quality,high purity nano powder.

In the present study characterization of ZnO nanoparticle has been done and its particle size is estimated by using XRD(Scherrer formula) .

2. EXPERIMENTAL

2.1 Co-precipitation method

In our work, ZnO nanoparticles were synthesized using chemical precipitation method. Using chemicals ; Zinc acetate dehydrate [$(CH_3COO)_2Zn.2H_2O$], Di- methylene sulphoxide(DMSO) and disttilled water ,Potassium hydroxide(KOH),thioglycero,lmethanol. The process of preparation of ZnO nanoparticles is shown below in figure1.

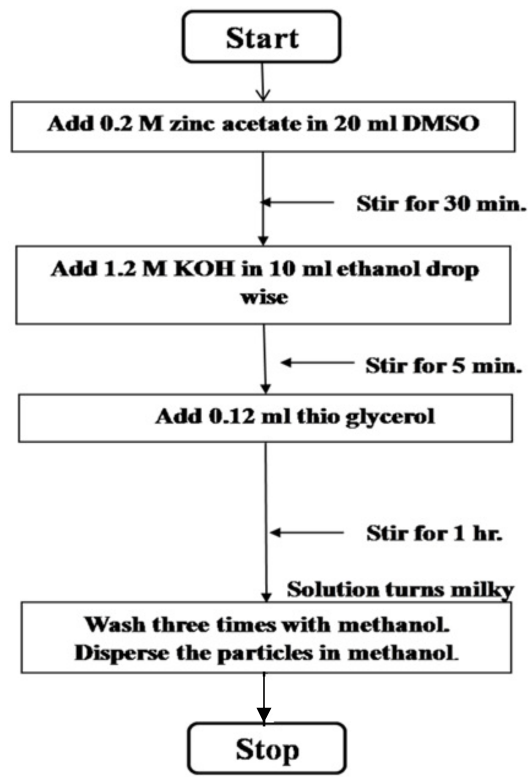

Fig 1:flow chart of preparation of ZnO nanoparticles.

The chemical reaction occurring during this process initiates the precipitation of ZnO nanoparticles precipitate was washed with 10ml methanol and filtered.The precipitate was dried and preserved in powder from.
Chemical reactions involved in preparation of ZnO nanoparticles:

$Zn\ (CH_3COO)_2 + KOH \rightarrow Zn\ (CH_3COO)(OH) + KCH_3COO$

$Zn\ (CH_3COO)OH + KOH \rightarrow ZnO + KCH_3COO + H_2O$

2.2 Characterization

The crystal structure of the synthesized particles was determined by X-ray diffraction (XRD, done on Bruker D-8 diffractometer) with Cu Kα radiation λ= 1.5406 Å,(40 kV, 40 mA).The corresponding particle size analysed using scherrer formula, shows the presence of nanocrystallites having size of 25 nm.

3. RESULTS AND DISCUSSIONS

At ambient pressure and temperature, ZnO crystallizes in the wurtzite (B4 type) Structure, shown in figure 2. This is a hexagonal lattice, belonging to the space group P63*mc*.

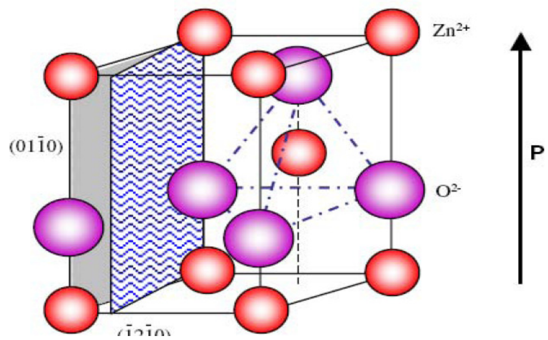

Fig 2: The Wurtzite Structure Model of ZnO. The Tetrahedral Coordination of Zn–O is shown

The structure of ZnOcan be simply described as a number of alternating planes composed of tetrahedrally coordinated O2- and Zn2+ ions, stacked alternately along the c-axis.[1] ZnO nanoparticles are successfully synthesized using precipitation method through chemical route.The X-ray diffraction patterns for the ZnO nanoparticles prepared is shown in Figure 3.

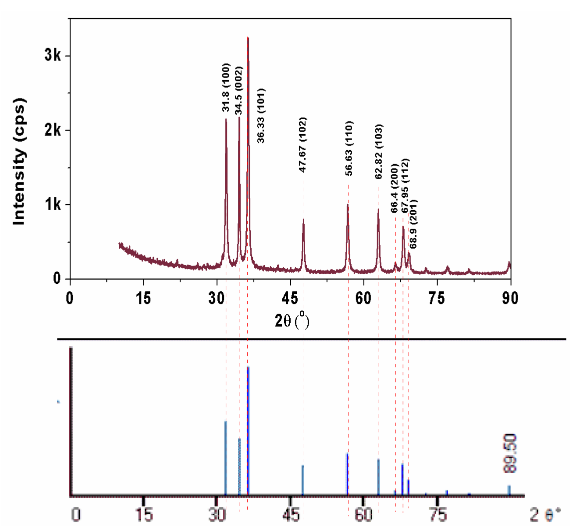

Fig 3: X-ray diffraction pattern of ZnO nanoparticles synthesized using precipitation method.

The sharp diffraction peaks of the synthesized products indicate their good crystallinity. The diffraction peaks in the XRD pattern exhibited hexagonal crystal structure of ZnO nanoparticles (JCPDS file number: 800075).

The ZnO nanoparticles have grown in polycrystalline nature, which is exhibited in the appearance of a number of XRD peaks attributed to different crystalline orientations.
The average crystalline size of the products was estimated from XRD peaks by using the following Scherrer equation (Cullity, 1978)

$$t = \frac{0.9\lambda}{B\cos\theta}$$

where t=particle size, λ is the wavelength of the incident X-ray beam, θ = the Bragg's diffraction angle, B=Full width at half maxima (FWHM) of the ZnO peak.
The calculated size of nanocrystallites was in the range of 19-36 nm.

4. CONCLUSIONS

ZnO nanoparticles were successfully synthesized using precipitation method through chemical route. In the present study, the nanoparticles show polycrystalline growth with small crystallites having sizes in the range of ~ 19-36 nm. These results show that the nanoparticles prepared using the above mentioned method can serve as a suitable host material for further experiments with doping.

AKNOWLEDGEMENTS

The authors would like to thank Director and Center director, UGC-DAE CSR, Indore (M.P.) for extending the XRD facilities. Authors are specially thankful to Dr. M. Gupta for his help in XRD measurements.

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