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DETERMINATION OF DEBYE TEMPERATURE AND SYNTHESIS OF ZINC OXIDE POWDER

L. Jithender*

Department of Physics, University Arts & Science College, Kakatiya University, Warangal-506 001, India.

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ABSTRACT

In this communication, we have been reported the synthesis and determination of thermal properties like Debye-Waller factor, Debye temperature and mean square amplitude of vibrations of zinc oxide (ZnO) powder by using chemical route and X-ray diffraction (XRD) technique respectively. After synthesis of the ZnO powder, the patterns of X-ray diffraction have been recorded. The Debye-Waller factor, Debye temperature and mean square amplitude of vibrations have been determined from integrated X-ray intensities. The intensities have been measured with a JEOL JDX-8P upgraded X-ray powder diffractometer fitted with a NaI(TI) scintillation counter using filtered CuKα radiation at room temperature and have been corrected for thermal diffuse scattering(TDS). The particle size has been estimated from Hall-Williamson plot and it has been found as 238 nm. The Debye temperature θ_M has determined as 350 K. The value of Debye temperature obtained in the present work has been compared with the value obtained from other methods. It is good agreed. The X-ray Debye temperature obtained in the present work has also been used to estimate vacancy formation energy (E_f) of ZnO powder.

Keywords: *Debye temperature, Chemical route synthesis, Particle size.*

1. INTRODUCTION

In the last few years the synthesis of powders of metal oxides has been reported by using different chemical methods viz. sonochemical, sol-vothermal, micro emulsion etc [1]. Gopi Krishna *et al.* [2, 3] were reported Debye temperature and mean square amplitudes of vibration of hcp rare earth metals. The Debye-waller factors and Debye temperatures of hcp Bi and Fe2O3 nanoparticle powders have reported by Jithender *et al.* [4, 5]. The fine particles of ZnO have deodorizing and antibacterial [6] properties and for that reason are added into materials including cotton fabric, rubber and food packaging [7, 8]. Recently, Christian O. Dimkpa *et al.* [9] evaluated the elative behaviour of metal oxide nanoparticles and microparticles in the plant environment to further understand whether Nps offer increased risks to plant growth and quality because of their smaller size. Consequently, CuO and ZnO NPs and MPs, and where relevant, Cu and Zn ions, were used in sand microcosms with and without growth of wheat. A novel approach to prepare ZnO nanowires with unique nanostructure by the thermal decomposition of the zinc carbonate hydroxide nanobelts, which are synthesized by the hydrolysis of zinc acetate aqueous solution in the presence of urea, has been given by Lu Ren *et al.* [10]. In the present paper, we have been reported the chemical route synthesis and determination of thermal properties like Debye-Waller factor, Debye temperature and mean square amplitude of vibrations of zinc oxide (ZnO) powder.

2. EXPERIMENTAL DETAILS

A chemical route synthesis technique has been used to prepare zinc oxide powder. 0.2 M of zinc acetate mixed in 20 ml DMSO (Di-methylene sulfoxide) and stirred for 30 minutes. Then added 1.2 M KOH (potassium hydroxide) in 10 ml ethanol drop wise in the solution. Again, stirred for 5 minutes. Then added 0.12 ml thio-glycerol to that solution and stirred for 1 hour. Finally, washed three times with methanol that dispersed the zinc oxide powder particles. The X-ray diffraction pattern has been recorded for this ZnO powder. The X-ray integrated intensities have been measured with an upgraded JEOL JDX-8P powder diffractometer fitted with a NaI(TL) scintillation counter using filtered CuKα radiation at room temperature. The X-ray tube was operated at 30 kV and 20 mA, and used goniometer with the speed of ½ ^{o} per minute. The X-ray intensities have been corrected for TDS (Thermal diffuse scattering) effect using the method Chipman and Paskin [11]. The XRD pattern of ZnO powder has been shown in Fig.1.

Corresponding author: L. Jithender
Department of Physics, University Arts & Science College, Kakatiya University, Warangal-506 001, India. E-mail: jitenderladal@gmail.com

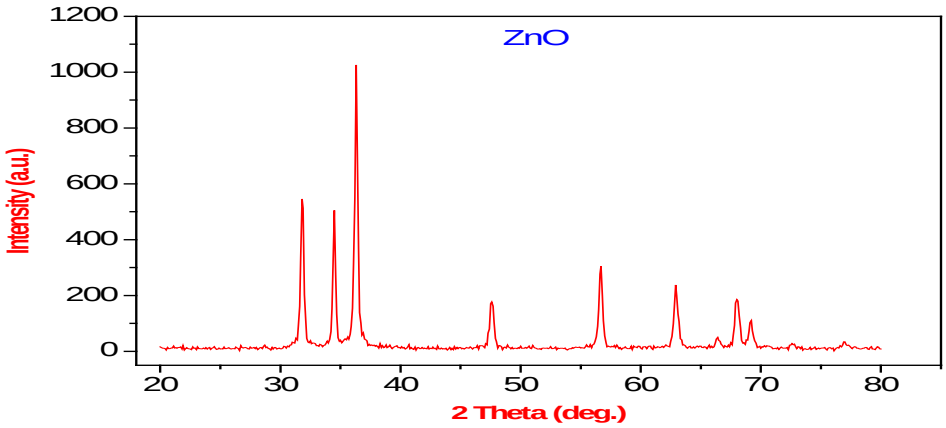

Fig. - 1. The X-ray diffraction patterns of zinc oxide powder.

3. ANALYSIS OF DATA

Zinc oxide metal powder has a hexagonal structure (hcp) [12]. The integrated intensity of Bragg reflection from a hexagonal cell may be written as follows [13-15]

$$Io = CIc \exp \{-(4\pi\sin\theta/\lambda)^2 [(<u_{II}^2> \cos^2\Psi + <u_{\perp}^2> \sin^2\Psi)]\} \quad (1)$$

where c is a constant, I_c is the calculated intensity. $<u_{II}^2>$ and $<u_{\perp}^2>$ refer to the components of the average vibrational amplitude projected onto the hexagonal axis and basal plane respectively. Ψ is the angle between the diffraction vector and the hexagonal axis and λ the wavelength. The calculated intensity I_c is given by

$$I_c = L_p J F^2 \quad (2)$$

where L_p is the Lorentz polarization factor, J the multiplicity factor and F the structure factor. The structure factor is given by

$$F^2_{hkl} = 36f^2 \cos^2 2\pi \quad \text{for} \quad -h+k+l = 3n \quad (3)$$

The structure factors are calculated from the atomic scattering factors given by Cromer and Waber [16]. These are corrected for anomalous dispersion [17]. $<u_{II}^2>$ and $<u_{\perp}^2>$ are obtained from a least square analysis of the logarithmic form of Eq. (1).

From these, the directional Debye-Waller factors $B_{\perp}$ and B_{II} are obtained from the equations.

$$B_{\perp} = 8\pi^2 <u_{\perp}^2>, \; B_{II} = 8\pi^2 <u_{II}^2> \quad (4)$$

The mean Debye-Waller factor B is given by

$$B = (2B_{\perp} + B_{II})/3 \quad (5)$$

The directional Debye temperatures $\theta_{\perp}$, θ_{II} and mean Debye temperature θ_M are obtained from $B_{\perp}$, B_{II} and B respectively using the Debye-Waller theory [18] relation

$$B = (6h^2/M k_B \theta_M) W(x), \; B_{\perp} = (6h^2/M k_B \theta_{\perp}) W(x), \; B_{II} = (6h^2/M k_B \theta_{II}) W(x) \quad (6)$$

where h is the plank's constant, k_B the Boltzmann constant, M the atomic weight and θ_M the Debye temperature. The function W(x) is given by

$$W(X) = [\phi(X)/X + (1/4)] \quad (7)$$

where $X = \theta_M/T$, T is the temperature of the crystal and $\phi(X)$ is the Debye function.

The values of W(x) for a wide range of X can be obtained from standard tables [19].

3. RESULTS AND DISCUSSION

In the present work, the particle size has been determined by measuring the (FWHM) full width at half maximum of the diffraction peaks rather than half widths. The particle size (t) has been estimated by using the Hall-Williamson method [12] and the equation is

$$B_r \cos\theta = k\lambda/D + \varepsilon \sin\theta \quad (8)$$

where B_r is the peak broadening due to crystallite size and ε the lattice strain, k the shape factor usually taken as 1.0 and D the crystallite size in nanometers, θ and λ are the Bragg angle and the wavelength of incident X-ray beam in nm.

The values of Debye temperature (θ), Debye-Waller factor (B) and amplitude of vibrations$\langle u^2 \rangle$ obtained in the present work have been compared with the values obtained from other methods [20]. This Debye temperature has been used to estimate vacancy formation energies for ZnO powder and the value is also included in Table 1. The values of E_f are not available for comparison.

Table - 1. Values of Mean square amplitude of vibrations, Debye-Waller factor, Debye temperature and vacancy formation energy of ZnO powder particles.

Parameter	Particle size (nm)	$\langle u^2 \rangle$ (Å^2)	B (Å^2)	θ_M (K)	(E_f) (eV)
ZnO	238	0.00414	0.32	350	0.27

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