International Journal of Advanced Research in Engineering and Applied Sciences

ISSN: 2278-6252
Impact Factor: 5.795

DETERMINATION OF DEBYE-WALLER FACTOR AND SYNTHESIS OF SILVER OXIDE POWDER PARTICLES FROM X-RAY DIFFRACTION AND COMBUSTION TECHNIQUE

L. Jithender*

Abstract: *In this paper, we have been presented the Combustion synthesis technique and determination of Debye-Waller factor, Debye temperature, mean square amplitude of vibrations and the particle size of silver oxide (AgO) powder particles. Combustion technique has been adapted to synthesis the AgO powder particles material using silver nitrate as oxidizer and glycine as fuel. X-ray diffraction study has been adapted to determine the solid state parameters like Debye-Waller factor, Debye temperature and mean square amplitude of vibrations and particle size of silver oxide powder particles. The integrated intensities have been recorded for this powder sample with 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 TDS (Thermal Diffuse Scattering) effect. Debye-Waller factor has determined as 0.22 $Å^2$. The particle size has been estimated from Hall-Williamson plot and it has been found as 294 nm. The Debye temperature has been determined as 366 K. The value of Debye temperature obtained in the present work has been used to estimate vacancy formation energy (E_f) of AgO powder particles. The Debye temperature value obtained in the present work has also been compared with the value obtained from other methods. The values of E_f are not available for comparison.*

Key words: *Combustion synthesis, Debye-Waller factor, Debye temperature, means squre amplitude of vibrations and particle size.*

*Department of Physics University Arts & Science College Kakatiya University Warangal, Telangana State, India.

1. INTRODUCTION

In the last few years, silver oxide powder particles have attracted the attention of many researchers because of its applications in oxidation catalysis [1], sensors [2], fuel cells [3], photovoltaic cells [4], all-optical switching devices and optical data storage systems [5] and hence silver oxide (Ag2O) is a versatile material [6]. Recently, the synthesis of powders of metal oxides has been reported by using different chemical methods viz. sonochemical, sol-vothermal, micro emulsion etc [7]. Zhouying Zhao et al. [8] and Kirk G. Scheckel et al. [9] have been reported the developed Ag/AgO_X nanostructure can potentially serve as an efficient system for multiple applications including catalytic chemicals, harsh environment gas sensing etc. and evaluated the aging of silver and zinc oxide nanomaterials in controlled Kaolin suspensions using X-ray absorption spectroscopy. Silver oxide powder was prepared by Combustion technique and the synthesis of oxide materials using redox compounds and mixtures [10]. Despite the fact, SCS being a very promising method, the work on Ag nanoparticle synthesis using this process, has been published by Poonam Sharma et al. [11]. They have reported the synthesis of the silver nanoparticles through SCS process by using two different fuels and varying their fuel ratio. The effect of different fuels, fuel to oxidant ratio has also been studied on morphology, structure and optical properties of the synthesized Ag nanoparticles. There was some work on Debye temperature and Debye-Waller factor for some metals and metal oxides in our laboratory [12,13]. S.Deshmukh *et al.* [14,15] were reported Debye temperature and mean square amplitudes of vibration of hcp rare earth metals. Recently, Christian O. Dimkpa *et al.* [16] 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. The parameter Debye temperature [17] represented the lattice vibrations present in tellurite glasses because it plays a vital role in the understanding of a large number of solid state problems connected with lattice vibrations or conduction process in semiconducting glasses [18-20]. The value of Debye temperature of pure TeO_2 glass was 249 K [21].This value is lower than the Debye temperature of pure SiO_2 (495 K) and that of BO_3 (276 K) [22], and P_2O_5 (307 K) [23]. In all the reports mentioned above, no attempt was made to calculate the X-ray Debye-Waller

factor that is a parameter of considerable interest. Motivated by the inexpensive Combustion synthesis and the interesting applications [6] of AgO powder particles, we have undertaken a systematic X-ray study to determine the solid state parameters like Debye-Waller factor (B), Debye temperature (θ_M), amplitude of vibrations $<u^2>$ and particle size (t) of AgO powder particles for the first time.

2. EXPERIMENTAL DETAILS

Silver nitrate (10g) and glycine (2.8g) were dissolved in 25 ml water contained in a beaker and placed on a hot plate for 15 minutes as the solution dehydrate to form a disposition like a gel. Then the beaker was placed in a preheated muffle furnace at 300° C. The solution boils, ignites with a flame and the entire reaction was completed within 5 minutes. The X-ray diffraction pattern has been recorded for these AgO powder particles. The integrated intensities have been measured for this powder sample with a JEOL JDX – 8P upgraded X-ray powder diffractometer fitted with a NaI (TI) scintillation counter using filtered CuKα radiation ($\lambda = 1.5418$ Å) at room temperature and have been corrected for TDS (Thermal Diffuse Scattering) effect by using the Chipman and Paskin method [24]. The XRD pattern of these powder particles has been shown in Fig.1. and the pattern confirms the formation of AgO. The XRD pattern of pure silver (Ag) is also shown in Fig.2.

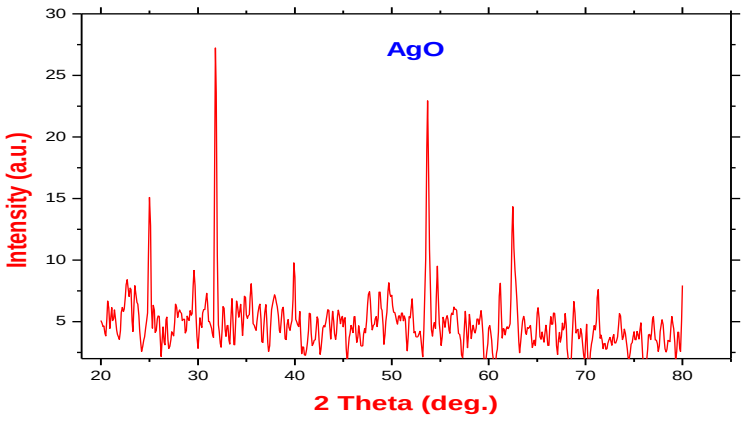

Figure 1. XRD pattern of silver oxide powder particles

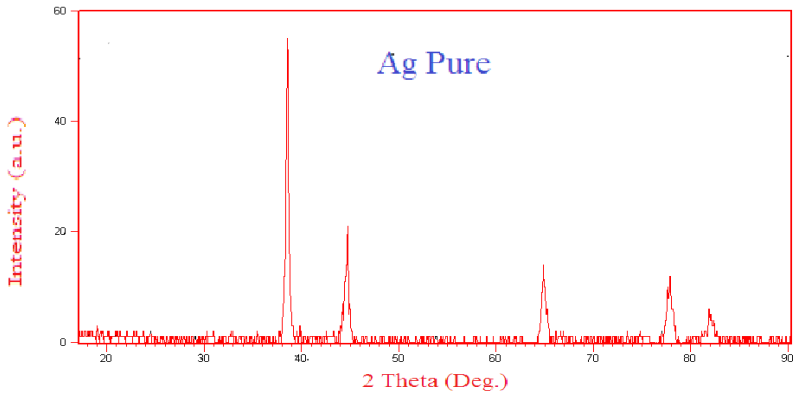

Figure 2. XRD pattern of pure silver powder particles

3. ANALYSIS OF DATA

Silver oxide metal powder has a hexagonal structure (hcp) [25]. The integrated intensity of Bragg reflection from a hexagonal cell may be written as follows [26-28]

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

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 □ 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 [29]. These are corrected for anomalous dispersion [30]. $<u_{II}^2>$ 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 [31] relation

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

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 [32].

4. RESULTS AND DISCUSSION

In this work, the values of Debye temperature (θ_M), Debye-Waller factor (B) and amplitude of vibrations $<u^2>$ have been measured for AgO powder particles. The Debye temperature has been used to estimate vacancy formation energy (E_f) also for the same sample. The E_f value is also included in Table.1. and there is no availability of comparison.

The particle size (t) has been estimated by using Hall-Williamson technique [33] and the equation is

$$Br \cos\theta = k\lambda/t + \varepsilon \sin\theta \quad (8)$$

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

Glyde [34] has derived a relation between the vacancy formation energy (E_f) and the Debye temperature (θ) of a solid. The relation is

$$E_f = A(k/\hbar)^2 M \theta^2 a^2 \quad (9)$$

where a is the interatomic spacing, A a constant shown to be equal to 1.17×10^{-2}, M the molecular weight and h and k are the Plank and the Boltzmann constants respectively. The validity of Eq. (9) was verified for a number of fcc, bcc and hcp metals [35]. There are no values of E_f available for comparison.

Table 1. Values of Debye temperature, mean square amplitude of vibrations and Debye-Waller factor of AgO powder particles

Parameter	Particle Size (t) (nm)	$<u^2>$ ($Å^2$)	B ($Å^2$)	θ_M (K)	E_f (eV)
AgO	294	0.00286	0.22	366	2.76

5. CONCLUSIONS

The Debye-Waller factor, Debye temperature, mean square amplitude of vibrations, vacancy formation energy and particle size of silver oxide (AgO) powder particles have been

determined for the first by using X-ray diffraction method. Combustion technique has been adapted to synthesis the AgO powder particles material. The Debye temperature of AgO powder particles has been used to estimate the vacancy formation energy (E_f). The value of Ef is also included in Table1.

REFERENCES

1. (a) Y. Chiu, U. Rambabu, M.-H. Hsu and H.-P. D. Shieh, J. Appl. Phys., 2003, 94, 1996; (b) D. M. Newman and P. Panchmatia, IEE Proc.: Sci., Meas. Technol., 2003, 150, 214; (c) F. Derikvand, F. Bigi, R. Maggi, C. G. Piscopo and G. J. Sartori, J. Catal., 2010, 271, 99; (d) W. Wang, Q. Zhao, J. Dong and J. Li, Int. J. Hydrogen Energy, 2011, 36, 7374.
2. (a) N. Yamamoto, S. Tonomura, T. Matsuoka and H. Tsubomura, Jpn. J. Appl. Phys., 1981, 20, 721; (b) V. V. Petrov, T. N. Nazarova, A. N. Korolev and N. F. Kopilova, Sens. Actuators, B, 2008, 133, 291.
3. E. Sanli, B. Z. Uysal and M. L. Aksu, Int. J. Hydrogen Energy, 2008, 33, 2097.
4. Y. Ida, S. Watase, T. Shinagawa, M. Watanabe, M. Chigane, M. Inaba, A. Tasaka and M. Izaki, Chem. Mater., 2008, 20, 1254.
5. W.-X. Li, C. Stampfl and M. Scheffler, Phys. Rev. B: Condens. Matter, 2003, 68, 165412.
6. Oscar A. Douglas Gallardo, Raquel Moiraghi, Micaela A. Macchione, Jorge A. Godoy, Manuel A. Pe´rez,* Eduardo A. Coronado and Vicente A. Macagno 2012 DOI: 10.1039/c2ra01044e
7. C.N.R.Rao, A.Muller and A.K.Cheetam (ends) The Chemistry anomaterials: Synthesis, properties and applications (Wenham: Wiley) (2004).
8. Zhouying Zhao and Michael A. Capenter, *J. Phys. Chem. C*, 117 (2013) 11132.
9. Kirk G.Scheckel, Todd P. Luxton, Amro M. El Badawy, Christopher A. Impellitteri and Thabet M.Tolaymat, *Environ. Sci. Technol.,* 44 (2010) 1312.
10. Kashinath C. Patil, Singanahally T.Aruna and S.Ekambaram, *Current Opinion in Solid State and Materials Science*, 2 (1997) 165.
11. Poonam Sharma • Gurmeet Singh Lotey • Sukhpreet Singh • N. K. Verma J Nanopart Res (2011) 13:2553–2561 DOI 10.1007/s11051-010-0148-3
12. L.Jithender, *International Research Journal of Pure Algebra*, 4 (2014) 528.

13. L.Jithender and N.Gopi Krishna, *Adv. Sci. Focus*, 1 (2013) 32.
14. N.Gopi Krishna, D.B. Sirdeshmukh, K.A. Gscheneidner Jr, Indian J. Pure & Appl. Phys., 26, 724, (1988).
15. N.Gopi Krishna, D.B. Sirdeshmukh, Acta Crystallogr., A 54, 513,(1988).
16. Christian O. Dimkpa, Drew E. Latta, Joan E. McLean, David W. Britt, Maxim I. Boyanov, and Anne J. Anderson, Environ. Sci. Technol., 47, 4734−4742, (2013).
17. R. El-Mallawany, Debye temperature of tellurite glasses, Phys. Stat. Solidi 130 (1992) 103.
18. M. Sayer, A. Mansingh, Transport properties of semiconducting phosphate glasses, Phys. Rev. B6 (1972) 4629.
19. G. Greaves, Small polaron conduction in V2O5±P2O5, J. Non- Crystalline Solids 11 (1973) 427.
20. B. Bridge, A. Higazy, Acoustic and optical Debye temperature of the vitreous system CoO±Co2O3±P2O5, J. Mater. Sci. 21 (1986) 2385.
21. E. Lambson, G. Saunders, B. Bridge, R. El-Mallawany, Elastic behaviour of TeO2 glass under uniaxial and hydrostatic pressure, J. Non-Crystalline Solids 69 (1984) 117.
22. J. Jackle, On the ultrasonic attenuation in glasses at low temperature, Z. Physica 257 (1972) 212.
23. B. Bridge, N. Patel, The elastic constants and structure of the vitreous system Mo-P-O, J. Mater. Sci. 21 (1986) 1187.
24. D. R. Chipman and A. Paskin, J. Appl. Phys. 30, 1998, (1959).
25. M.J. Buerger, X-ray Crystallography (John Wiley and Sons, New York), P.68.
26. M. Blackman, Acta Crystallogr., (Denmark) 9 1956,734.
27. H. Lipson, International Tables for X-ray Crystallography, (Kynoch Press, Birmingham) Vol.2 1959.
28. R.W. James, The Optical Principles of the Diffraction of X-rays (Bell and Sons, London.) 1967.
29. D.T. Cromer and J.T. Waber, Acta Crystallogr. (Denmark), 18 1965, 104.
30. R.W.G. Wyckoff, Crystal Structure, (John Wiley & Sons, New York) Vol.1, 1963.
31. D.T.Cromer and D. Liberman, J. Chem. Phys., 53 1970, 1891.

32. G.C. Benson and E.K.Gill, Tables of Integral Functions related to Debye-Waller factors (National Research Council of Canada, Ottawa.) 1966.
33. R.Bharathi Rehani, P.B. Joshi, N.Kirit Lad and Arun Pratap, *Indian J. Pure Appl. Phys.*, 44 (2006) 157.
34. H. R. Glyde, *J. Phys. Chem. Solids (GB)*, 28 (1967) 2061.
35. Tewary.V.K. (1973): J.Phys.F (GB), 3,704.